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THE COLLEGE OF EARTH AND MINERAL SCIENCES

FUELS AND COMBUSTION LABORATORY

PLANE FLAME FURNACE COMBUSTION TESTS ON JPL-DESULFURIZED COAL

Contractor's Report Number: PSU-FCL-C-82-345

Final Technical Report

Dr. James J. Reuther, Assistant Professor of Fuel Science and Principal Investigator
and

Mr. H. T. Kim and Mr. J. G. H. Lima, Graduate Assistants in Fuel Science

May 15, 1982

JPL Contract Number: 956123

Contractor:
The Pennsylvania State University
207 Old Main Building
University Park, PA 16802



This work was performed for the Jet Propulsion Laboratory, California Institute of Technology, sponsored by the U.S. Department of Energy through an agreement with the National Aeronautics and Space Administration.

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**The Pennsylvania
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The Pennsylvania State University
Fuels and Combustion Laboratory

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ABSTRACT

The program objective was to reliably determine, under the well-defined and well-controlled simulated boiler combustion conditions generated by The Pennsylvania State University Fuels and Combustion Laboratory plane flame furnace, the combustion characteristics of: (a) three raw bituminous (PSOC-282 and 276) and subbituminous (PSOC-230) coals; (b) the raw coals partially-desulfurized (ca.-60%) by "JPL-chlorinolysis"; and (c) the "chlorinated" coals more completely desulfurized (ca.-75%) by "JPL-hydrodesulfurization," in order to establish to what extent the combustion characteristics of the untreated coals were altered upon JPL-sulfur removal.

The plane flame furnace was preheated to 900°C and fired at 10^4 Btu/hr and at $\pm 20\%$ excess air. Residence times of 1-2 seconds, peak flame temperatures of 1400-1500°K, and heating rates of 10^4 K/sec, typical of utility boilers, were simulated.

Upon decreasing the parent coal volatile matter generically by 80% (from 36.6 to 6.8%) and the sulfur by 75% via the JPL desulfurization process, ignition time was delayed 70-fold, burning velocity was retarded 1.5-fold, and burnout time was prolonged 1.4-fold. Total flame residence time increased 2.3-fold.

The JPL desulfurization process appears to show significant promise for producing technologically combustible and clean-burning (low-SO₂) fuels

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1. INTRODUCTION

As background to this final report entitled, "Plane Flame Furnace Combustion Tests on JPL-Desulfurized Coals," the following historical account of the Jet Propulsion Laboratory-sponsored program at The Pennsylvania State University Fuels and Combustion Laboratory (PSU-FCL) should prove informative. On May 5, 1981, Dr. John J. Kalvinskas, Project Manager-Coal Desulfurization of the Jet Propulsion Laboratory (JPL) contacted Prof. William Spackman, Director, PSU Coal Research Section, about the possibility of conducting independent combustion tests on high-sulfur coals that had or had not been subjected to a JPL-patented desulfurization process [1]. Dr. Kalvinskas was then referred to Dr. James J. Reuther, Assistant Professor of Fuel Science, whose primary research interest at PSU is combustion. Following that telephone conversation, and the submission and approval of an informal preproposal by Prof. Reuther of PSU and Dr. Kalvinskas of JPL, respectively, an official proposal was submitted by Prof. Reuther to the JPL on May 20, 1981. A copy of this proposal (PSU-FCL-C-81-137) is included in this Final Report as Appendix I. As that document states, Prof. Reuther proposed a 6-month plane flame furnace combustion test program on JPL-desulfurized coal for the period of 7/1/81-12/31/81. This contract period was decided upon by Prof. Reuther because it most satisfactorily accommodated the immediate needs of the JPL while at the same time did not disrupt other sponsored-research being conducted with the PSU-FCL plane flame furnace solid fuel combustion test facility. On August 21, 1981, Dr. Kalvinskas telephoned Dr. Reuther to inform him that preliminary funding for the program was approved and that the contract was in procurement. On September 15, 1981, official copies of the formal contract were received by The Pennsylvania State University. On November 13, 1981, Contract No. 956123 was signed on behalf of The Pennsylvania State University Office of Sponsored Programs, W. D. Moir, Director. On November 23, 1981, completely executed (by JPL) copies of the contract were returned to PSU. Hence, November 23, 1981, became the official "Date of Contract," with June 8, 1982 becoming the completion date. Prof. Reuther and Dr. Kalvinskas were named PSU Principal Investigator and JPL Technical Manager, respectively.

The reason for presenting this historical narrative is because of a statement in "Article 2: Delivery or Performance Schedule" of Contract No. 956123 that reads: "Time is of the essence in the performance of this Contract." Prof. Reuther has fully appreciated this need on the part of JPL to execute first-class combustion tests on JPL-desulfurized coals with dispatch, and to do within the somewhat limited budget. In order to satisfy these simultaneous needs for speed, accuracy, and economy, and in an attempt to satisfactorily reschedule the use of the PSU-FCL plane flame furnace combustion test facility -- given the somewhat disrupting 6-month delay in the execution of the original contract (see Appendix I) -- Prof. Reuther had little choice but to arrange for all the solid samples extracted from JPL-coal flames generated by the plane flame furnace to be analyzed in one batch. Hence, the technical reports required (Article 2:C(1) of the Contract) after completion of combustion testing of each batch

of coal sample have become one report, this one. Because this document sets forth the results of all tests required in the Contract, it represents the Final Report. Moreover, it should be noted and appreciated that the decision by Prof. Reuther to conduct the JPL Contract in the stated fashion has resulted in the combustion tests, data reduction and interpretation, and final report drafting to be completed fully one-month ahead of the scheduled completion date without sacrificing quality and without going over budget. The reasons for these rather significant accomplishments, which the JPL should recognize, are nothing less than sheer dedication and very hard work on the part of Prof. J. J. Reuther, Principal Investigator, and of Mr. H. T. Kim and Mr. J. G. H. Lima, Graduate Assistants in Fuel Science, to see that the proposed research program was executed in a completely professional and expeditious way.

In the interests of communicating the complete combustion test results to Dr. Kalvinskas as soon as they were available, Prof. Reuther sent to him at the JPL a document (PSU-FCL-C-82-346) containing a table of Contract-required data (and more). A copy of this letter is given in Appendix II. This report more fully explains and interprets these combustion test data on JPL coals.

2. TECHNICAL DISCUSSION

2.1. Contract Objective

The purpose of the research program, entitled, "Plane Flame Furnace Combustion Tests on JPL-Desulfurized Coals," was to reliably determine, under well-defined and well-controlled simulated boiler combustion conditions, the combustion performance characteristics (ignition times, burning velocities, and burnout times) of three (3) samples of raw (as received) bituminous (PSOC-282 and 276) and subbituminous (PSOC-230) ranks of coal, three (3) samples of the same raw coals partially desulfurized (ca. -60%) by a Jet Propulsion Laboratory (JPL) "chlorinolysis" process, and three (3) samples of these "chlorinated" coals more completely desulfurized (ca. -75%) by a more severe JPL-patented "hydrodesulfurization" process, in order to establish to what extent the burning characteristics of the untreated coals were altered upon sulfur removal.

2.2 RESEARCH TASKS

2.2.1. Work Statement

The nine (9) listed samples of pulverized coal with diminishing sulfur content were fired in The Pennsylvania State University Fuels and Combustion Laboratory plane flame furnace, shown schematically in Figure 1. This intermediate-scale laboratory device essentially simulates the combustion environment in a utility boiler: residence times of 1-2 seconds; peak gas temperatures of 1400-1500°K; heating rates of 10^4 °K/second. Because the furnace design produces a one-dimensional flame, fuel particles experience a nearly identical time/temperature history as they vertically traverse the combustion zone. Flat flames stabilize at different positions downstream of the fuel entry plane primarily because of different compositional properties of the solid pulverized fuel, such as the volatile matter, hydrogen, and fixed-carbon contents. It was the effect of the alteration of these three fuel properties upon JPL-desulfurization (decrease, decrease, and increase, respectively) on raw coal burning characteristics that was determined in this program.

To fully understand the design and operation of the plane flame furnace combustion test facility, the following narrative has been prepared.

2.2.2. Plane Flame Furnace: Description

Figures 1, 2, 3, and 4 schematically illustrate components and the general design of the furnace that has been extensively used at The Pennsylvania State University Fuels and Combustion Laboratory for studies of combustion on pulverized fuel flames. This furnace was designed to give safe operation for pulverized coal premixed with cold air to produce a plane flame, that is, a residence time distribution corresponding to close to plug flow with no back-mixing into the flame. Essentially, the furnace consists of a pulverized fuel-air premixer and burner, a down-fired vertical combustion chamber, and an uprising refractory leg connected to a steel stack.

The premixer-burner is situated on the top of the combustion chamber. It receives the mixture of fuel plus primary conveying air, mixes it thoroughly with the secondary air, and disperses the mixture in a plug flow manner. The shape of the premixer-burner is a truncated pyramid of square cross-section whose base is fitted into a two row bank of water-cooled copper tubes. The pyramid expands downwards with an angle 20.6° between the center line and its sides. The dimensions of the base resting on the top of the water-cooled tubes are 6.5"x6.5". The pyramid is constructed of stainless steel plates which are bonded together with high temperature air-setting mortar (Franset, J. H. France Co.). The pyramid is easily removable for inspection of the interior of the furnace.

The water tube bank consists of two rows of horizontal tubes. The tubes in each row are one outside tube diameter apart and rows are separated vertically by about one inch. The top of each tube is fitted with a stationary vane of triangular cross-section that tapers from base width equal to the outer diameter of the tube to a sharp peak located about one inch above the center line. The vanes prevent the accumulation of pulverized fuel dust on the top of the tubes and direct the flow of fuel particles through the bank with minimum turbulence. The two rows of tubes are staggered in such a fashion that the empty spaces between the tubes in a row are in exact vertical alignment with the tubes of the other row. This arrangement makes the tube bank function as an efficient radiation shield, yet still allows the fuel particles to pass through. The water-cooled tube bank forces the flame to stabilize at the desired position and it prevents the flame from flashing back into the premixing zone. The tubes are of $\frac{1}{2}$ " thick copper wall while the vanes are constructed of 24 gauge galvanized sheet soft silver soldered onto the tubes. Water flow is commenced before the furnace is fired, obviously, and maintained at the end of a test until the furnace is cool, to prevent melting of the silver solder.

The combustion chamber consists of four vertical walls constructed of insulating refractory bricks, bonded together with high temperature mortar. The bricks are composed of 50% alumina and 50% silica, and can withstand up to 1530°C temperature. The height of the vertical combustion chamber is approximately 325 cm, interior cross-section area is 6.5" square (16.51 cm), and the thickness of the walls is 5" (12.7 cm). The height of the combustion chamber was recently

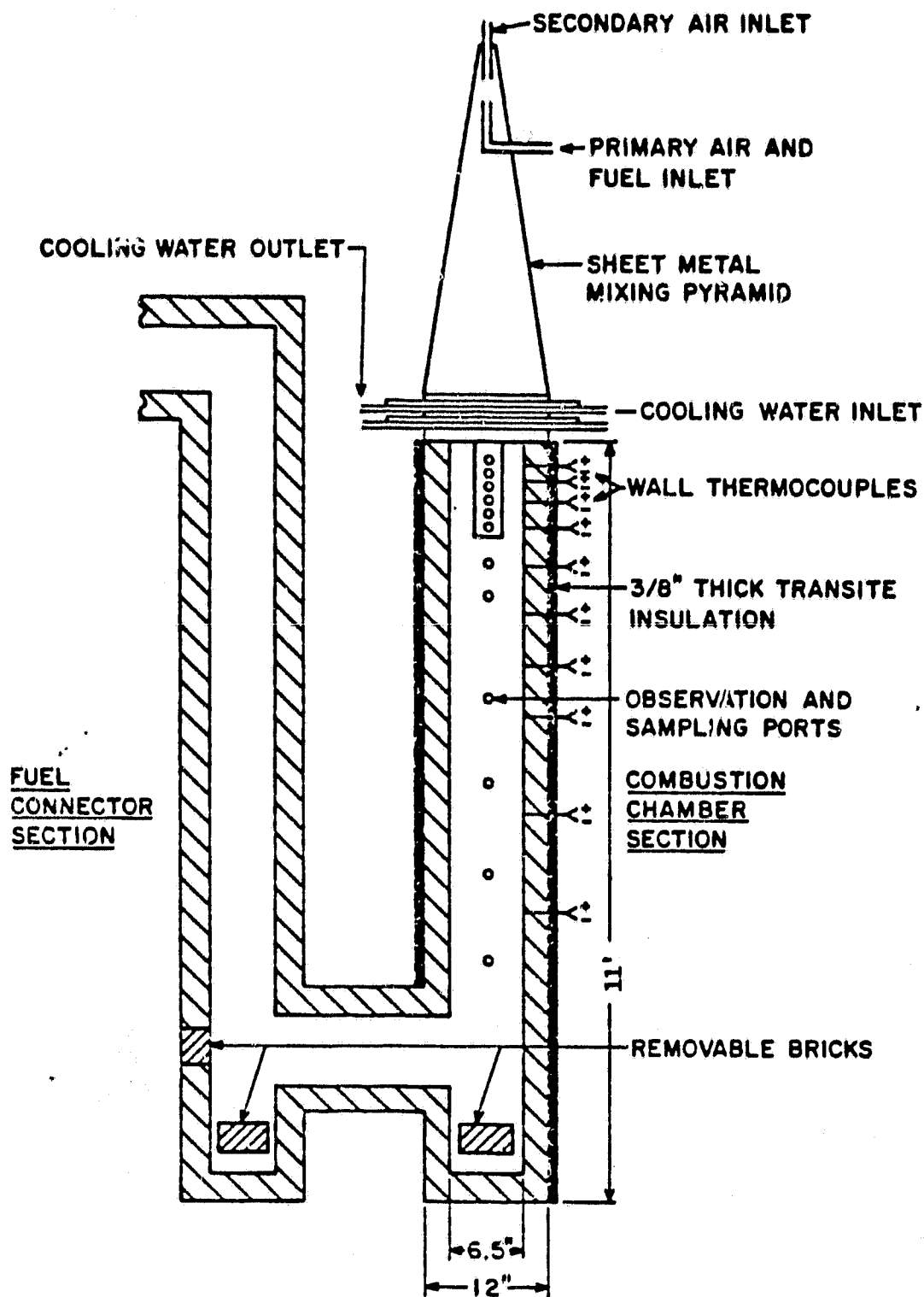


Figure 1. Plane Flame Furnace Schematic

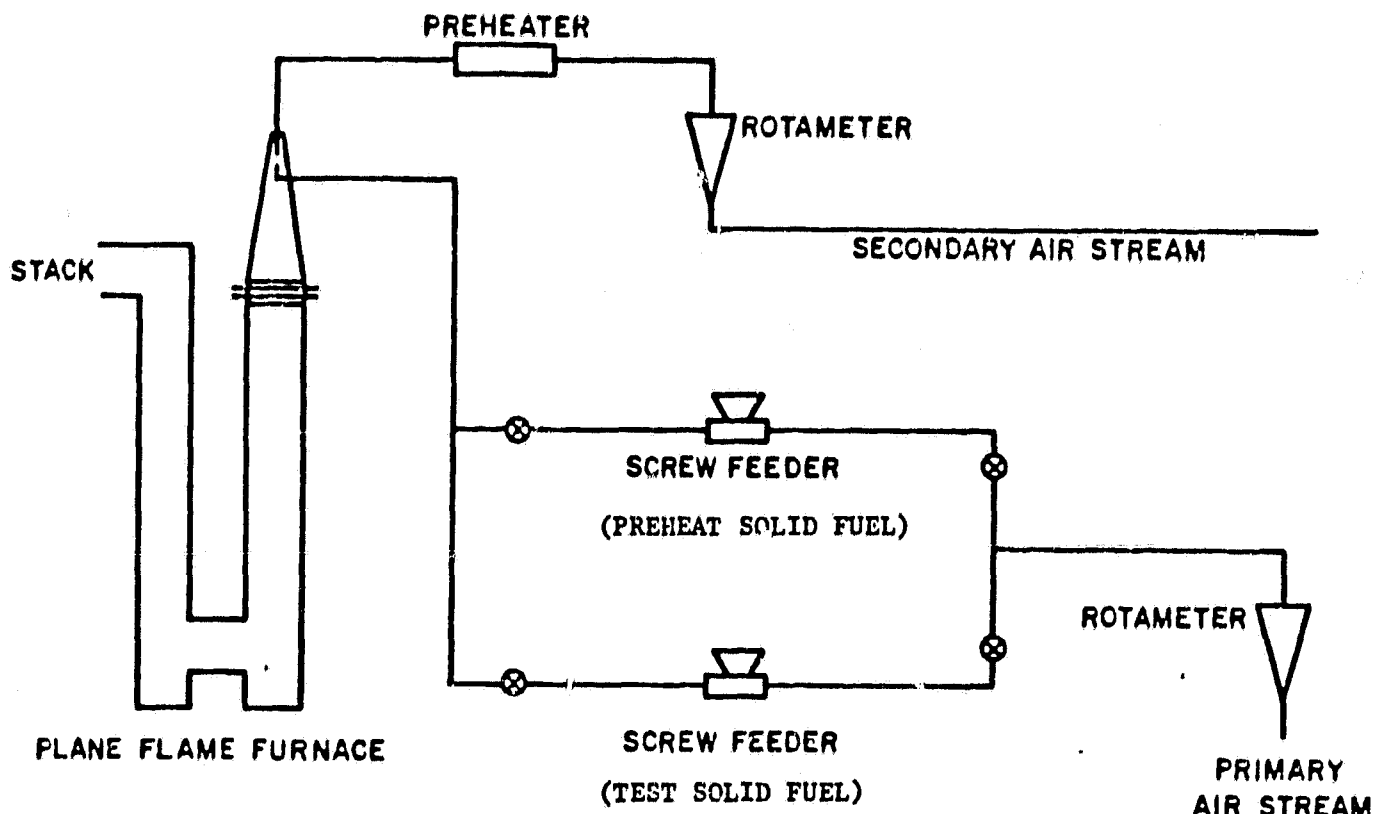


Figure 2. Diagram of Plane Flame Furnace Feeder System

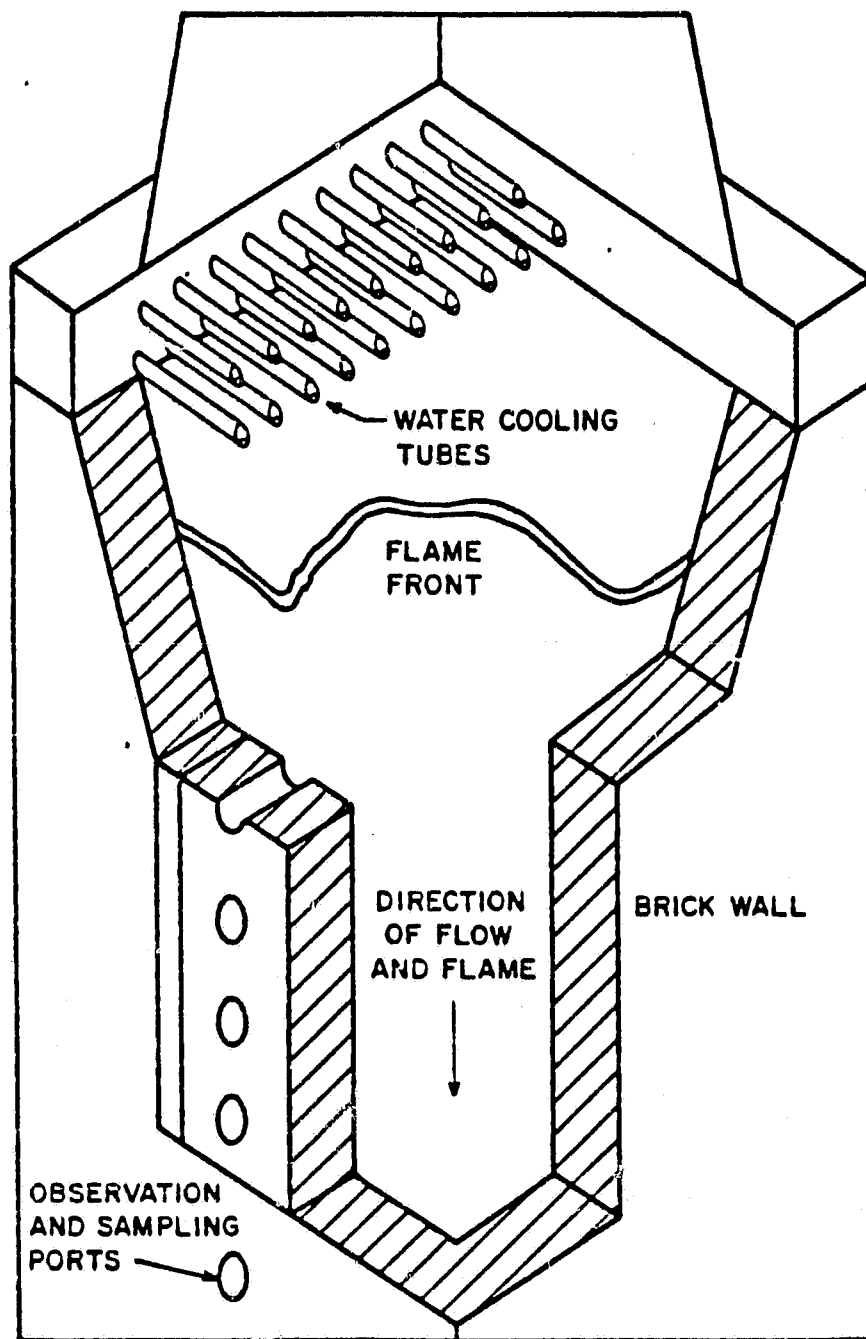
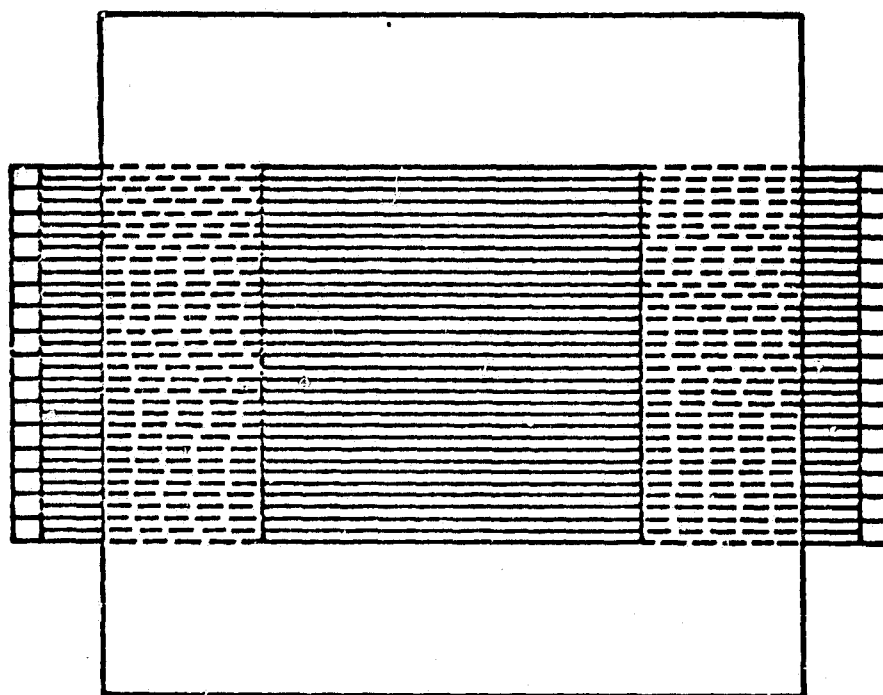
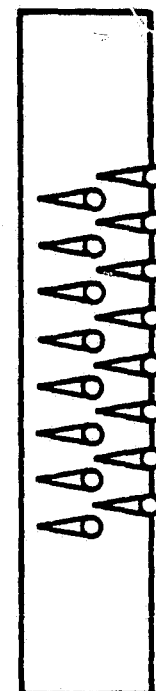


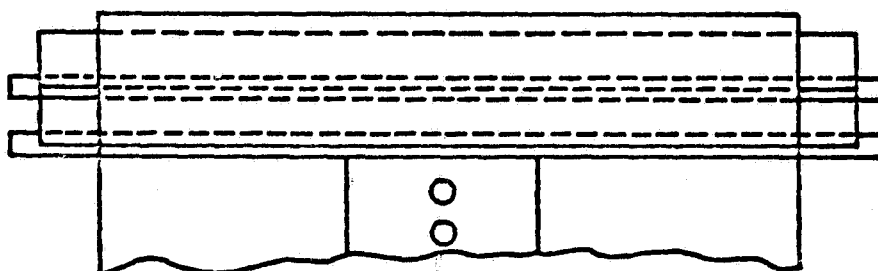
Figure 3. Section Showing Water-Cooled Flame Stabilizer



TOP VIEW



SIDE VIEW



FRONT VIEW

Figure 4. Detail of Cooling Water Tubes

increased from 226 cm to 335 cm to achieve longer particle residence time, and the wall thickness was increased from 6.35 to 12.7 cm to reduce heat loss. The combustion chamber is encased with 3/8" thick transite sheet to reduce heat loss and eliminate air leakage.

All but one of the sampling ports on the front side wall of the furnace are kept closed during the furnace operation using ceramic plugs. The junction between the uprising flue and the combustion chamber is located at a short distance above the bottom of the chamber in order to collect product material at the base. The flue is constructed of the same type of bricks and mortar as used for the combustion chamber, but are a single layer thick (6.35 cm).

The air supply system consists of a primary air line and a secondary air line. The primary air line supplies compressed air (80 psi) for the pulverized fuel ejector (see later) and the secondary air line supplies low pressure air, produced by a blower with a capacity of 350 SCFM. A 2" gate valve in the secondary air line controls the flow of air. The primary and secondary air lines are connected to two rotameters (Schulte and Koerting Co., 0-25 SCFM, 0-30 SCFM), respectively. The total flow rate of combustion air is controlled by adjusting the required total flow through both primary and secondary air lines.

The pulverized fuel feeder system consists of a large primary hopper, a small secondary hopper, a vibratory feeder, and a venturi ejector for introducing the fuel into the primary air, which is then pneumatically carried to the premixer-burner. The venturi device is composed of a funnel whose spout is fitted into the throat of a asymmetric venturi. The funnel is made out of brass and the venturi is made by cutting and sealing a notch in a 3/8" stainless steel tube. The upstream and downstream of the notch are cut at angles respectively of 60° and 12° to the axis of the tube, and to a depth of about 2/3 of the diameter of the tube. The funnel is soldered into an opening left in the throat of the venturi. With the unit installed in the primary air line, the flow through the venturi creates a suction at the spout of the funnel which is sufficient to allow pulverized fuel to be pulled from the funnel into the air line by atmospheric pressure.

Figures 5 and 6 show the details of the feeder. It consists primarily of a commercially-obtained SCR-20 Vibra-Screw Feeder. The maximum deviation in feed rate from the mean value during a given run is typically only ±5%.

Before the start of a test, the steel stack is heated with a gas burner located at the base to create natural draft conditions (30-45 minutes). During this time, the feeder is calibrated by collecting test fuel over timed periods and weighing it.

The furnace is raised in temperature before the start of firing with coal by means of a water-cooled gas burner (see Figure 7) inserted in the top of the furnace below the tube bank. A small gas flame is used initially, with a low air flow through the tube bank, and

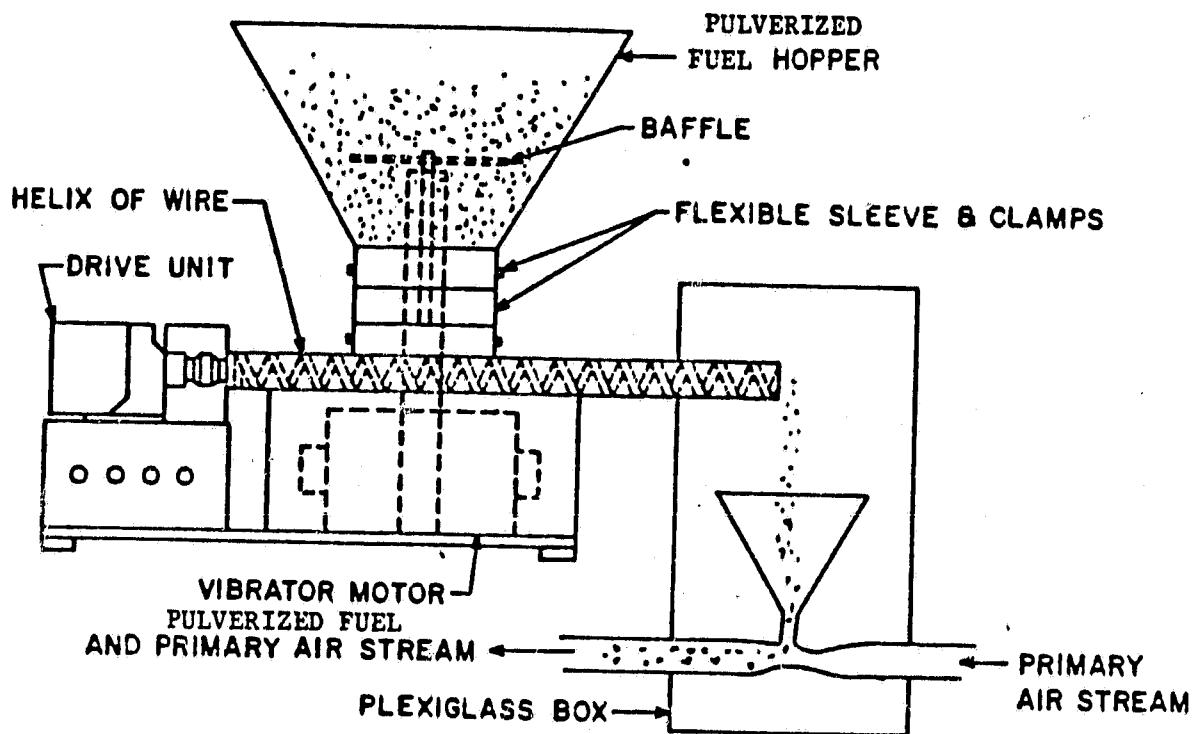


Figure 5. Diagram of Vibrating Screwfeeder System

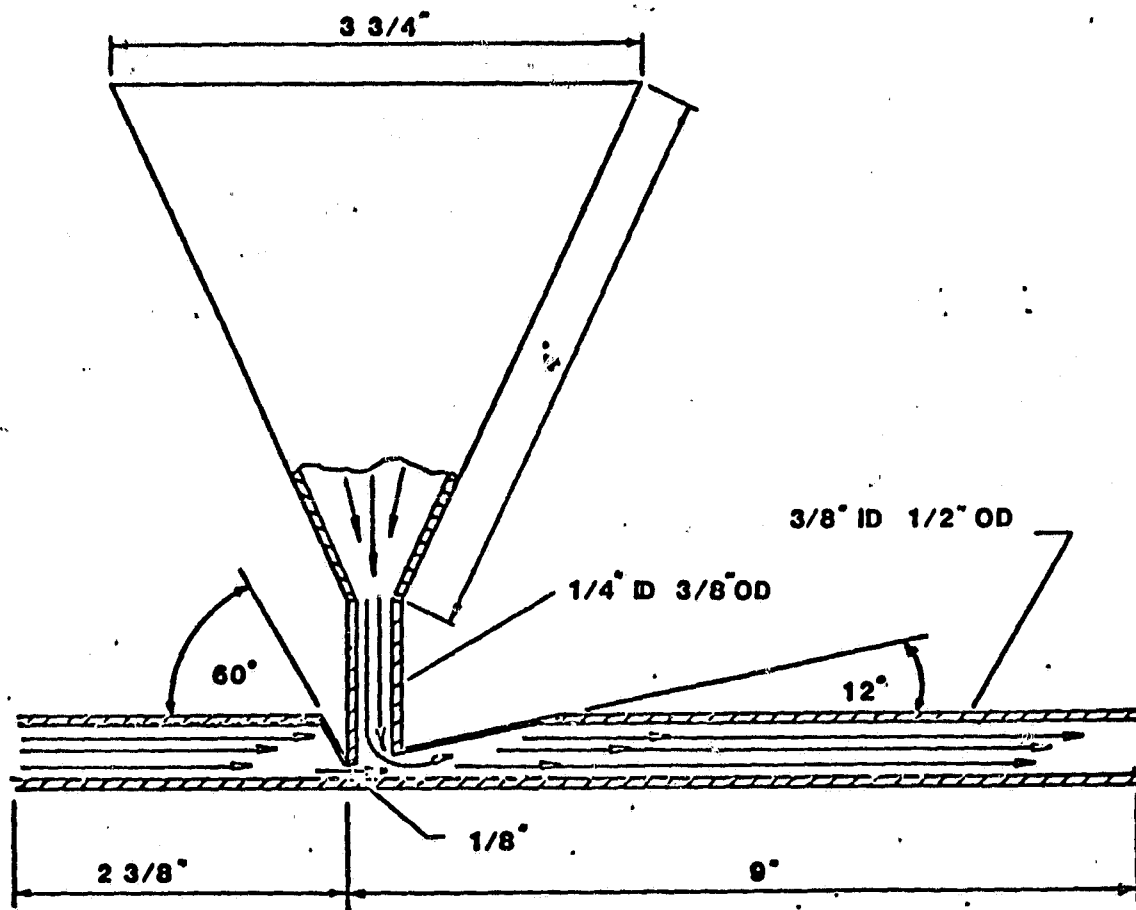


Figure 6. Details of ejector.

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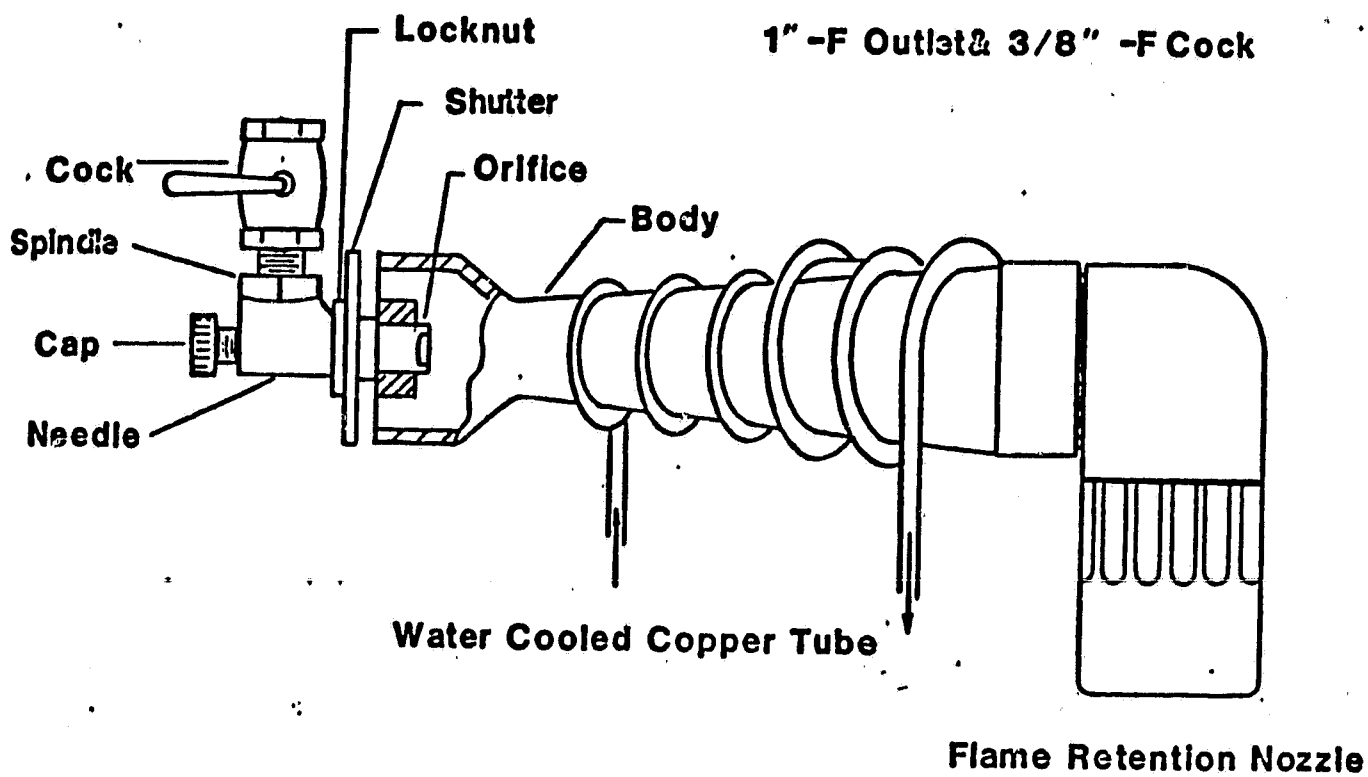


Figure 7. Gas burner.

as the furnace enclosure becomes hotter, more gas and air are supplied at a rate less than flame failure, until full burner capacity is reached. More will be said about the ignition procedure required for determining fuel ignition temperature in Section 2.3.2.1.

The following precautions were considered important for safe and correct furnace operation:

1. The pulverized fuel feed rate must be recalibrated for each type of fuel used.
2. The funnel attached to the venturi should be checked periodically, since blockage of the nozzle can occur because of larger fuel particles or foreign material.
3. Before the furnace is fired, water must be passing through the water tube banks.
4. The furnace wall temperature must be checked periodically to confirm the presence of the flame.
5. Material must be removed every 30 minutes from the bottom of the furnace and stack, in order to prevent pressure build-up in the furnace.
6. Before any actual test is conducted, steady state temperature must be obtained.
7. After the experiments are finished, the air and feeder lines must be first turned off. The water, however, must run through the water tube banks for the following night so that the furnace may cool down without damage to the mixer-burner.
8. The high pressure gas line must be turned off at the main.

2.2.3. Plane Flame Furnace Diagnostics: Description

The measurement of wall and gas temperatures, and the collection of gas and solid samples require the construction of special purpose probes, which has been done. The designs are shown schematically and discussed briefly.

2.2.3.1. Wall temperatures: Thermocouples

In order to measure the furnace inner-wall temperatures, twelve thermocouples are connected to a 24-point Esterline Angus (Model E1124E) temperature recorder that scans the twelve thermocouples once every 24 seconds. The thermocouples are fixed along the longitudinal center-line of the right side of the combustion chamber. The positions of the wall thermocouple stations are shown in Figure 1. The thermocouple wire (0.128" diameter Pt/Pt-10% Rh) is insulated with alumina double-bore tubing (.0126" O.D. x 0.0233" I.D. x 6" long) and installed in an alumina protecting tube (0.218" O.D. x 0.150" I.D. x 6" long) with one end closed.

2.2.3.2. Gas Temperatures: Suction Pyrometer

Furnace gas temperatures are measured with a water-cooled suction pyrometer, with which flue gas is pulled at high velocity over a shielded thermocouple, as shown in Figure 8. It consists of a Pt/Pt-10% Rh thermocouple that is placed into a two-bore ceramic tube. The head of this tube is protected by another ceramic tube (O.D. 19"/64, I.D. 13"/64 and 8" long) with one end closed. This whole assembly is covered by an open-ended ceramic shield tube and gas is withdrawn through the annulus. This head is supported on a water-cooled body composed of two concentric copper tubes through which water is circulated to cool the hot gases after they have passed the thermocouple head. The suction pump has a capacity of 0.2 CFM.

2.2.3.3 Wall-Gas-Temperature Correlation

Figure 9 shows how axial furnace wall temperatures, as measured with thermocouples, compare with gas temperatures, as measured with the suction pyrometer.

2.2.3.4. Gaseous Combustion Products: Gas Sampling Probe

The probe used for collecting gas samples from a pulverized-fuel flame must meet the following basic requirements: (a) it has to be sufficiently cooled to protect the probe from thermal destruction and to quench the sample rapidly; (b) it has to be small enough that its presence does not significantly affect the flow conditions of the flame; (c) it has to be completely sealed to prevent leakage of air into the sampling system or furnace; and (d) it has to be capable of separating the gaseous sample from the solid material. The gas sampling probe used for the JPL desulfurized coal combustion tests is shown in Figure 10. The probe is water-cooled, and the sample enters through a nozzle that is directed upstream, parallel to the flow. It turns a 90 degree bend and then travels through a 0.2 inch

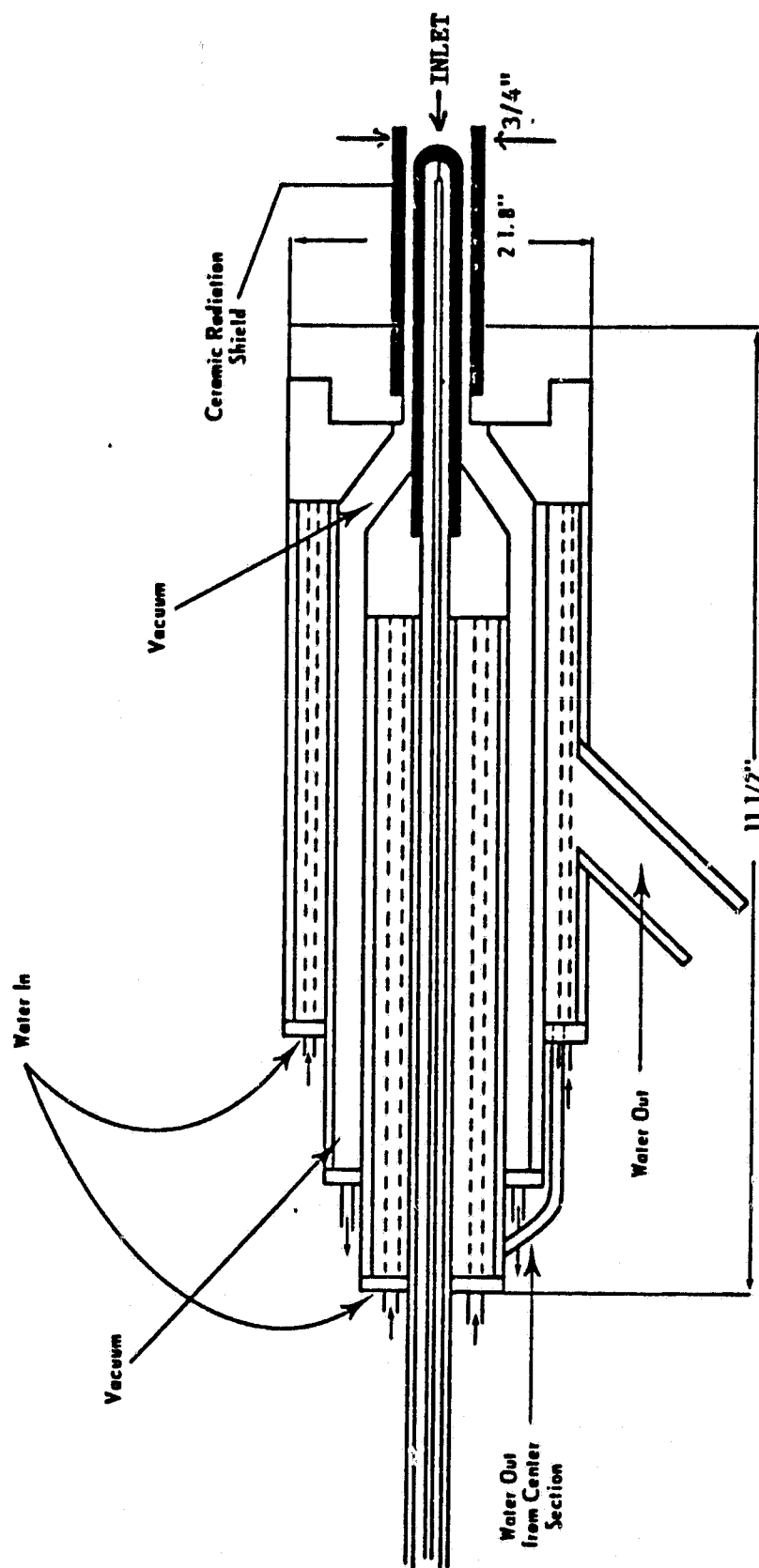


Figure 8. SINGLE SHIELD SUCTION PYROMETER FOR FLAME TEMPERATURE

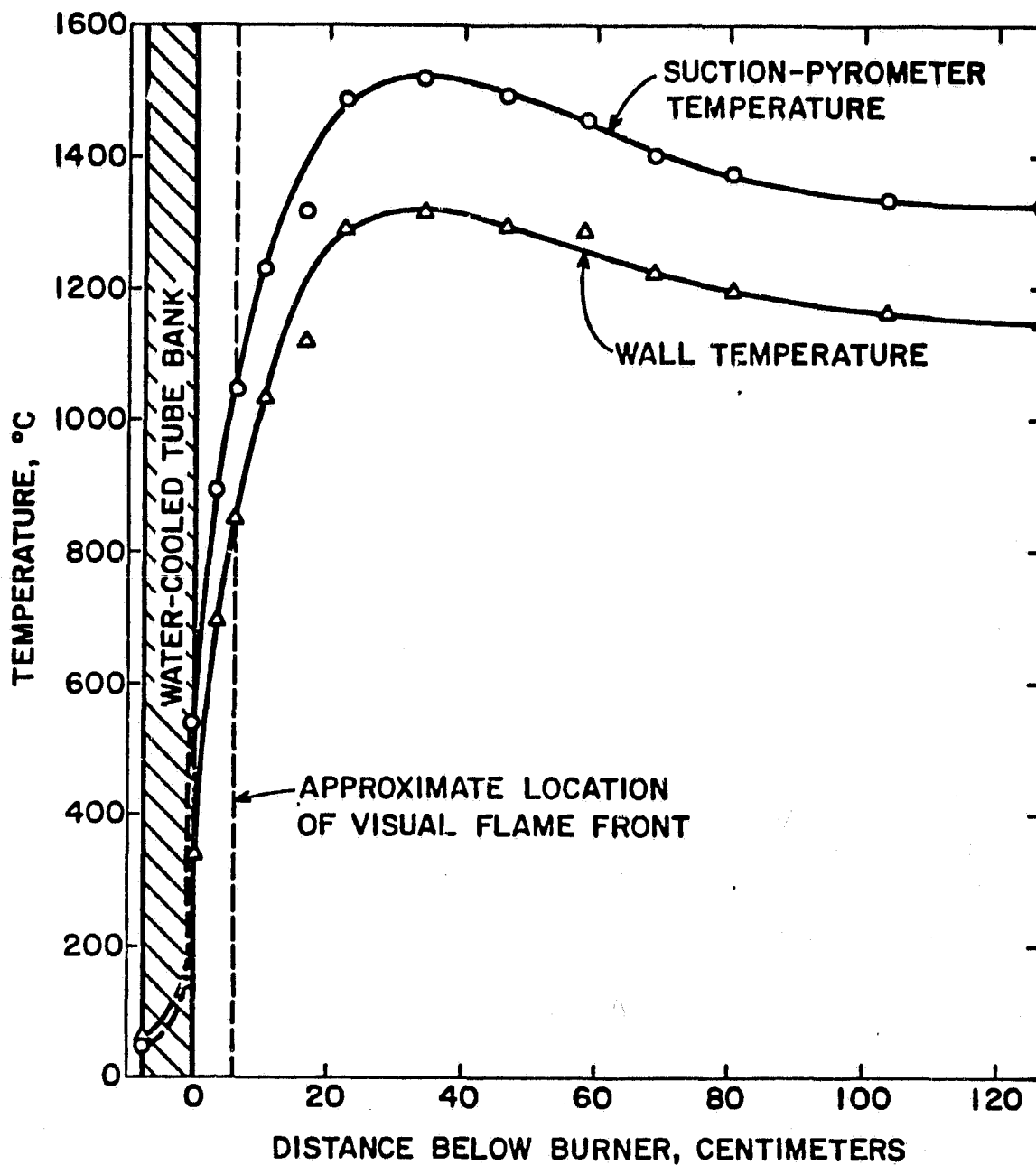


Figure 9. Temperature profiles in the plane flame furnace.

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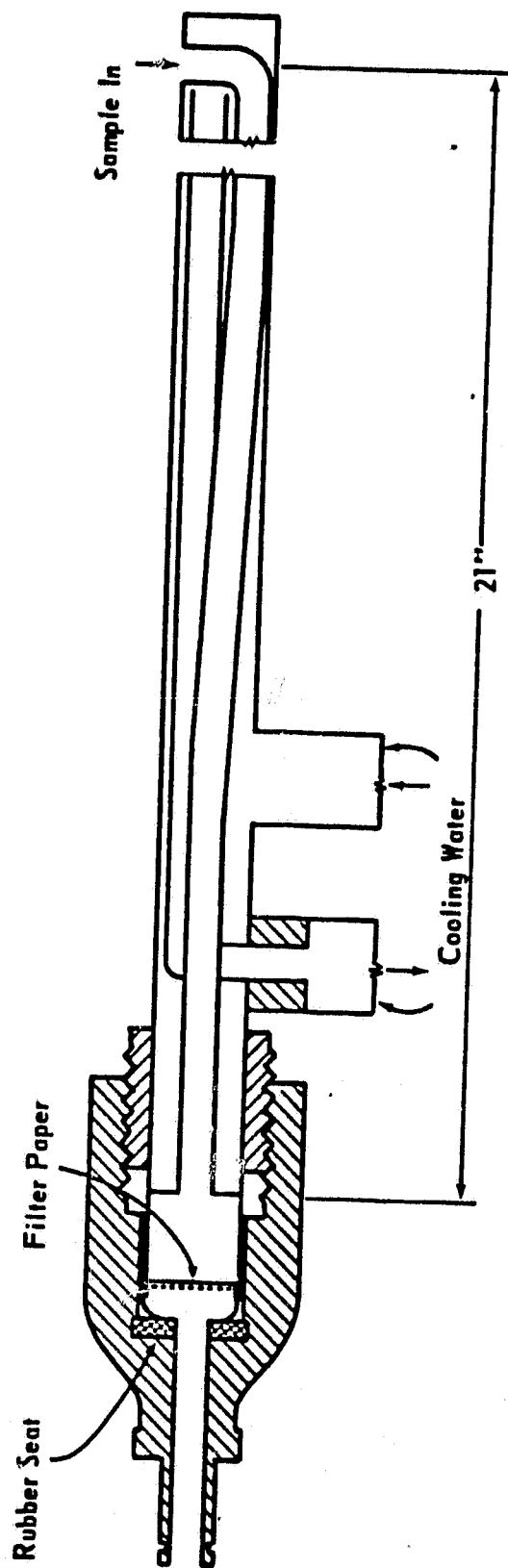


Figure 10. GAS-SAMPLING PROBE

inner diameter copper tube to the filter chamber where the solid material is completely removed. The sample is collected by inserting a standard gas collection bulb in line just downstream from the exit of the probe. Heat transfer is very good in the small diameter tube, thus, the gas sample is very rapidly cooled. The filter chamber, that uses a small filter-paper disc (0.625 inch) supported by a wire screen, is easily taken apart for cleaning.

Gaseous products of combustion sampled at various distances down the axis of the furnace are analyzed via two techniques: (i) batch, using a gas chromatograph (Carle Series-S-157A Random Access GC), that provides separation of H_2 , O_2 , N_2 , CO , CO_2 , H_2S and 20 various hydrocarbons, or (ii) on-line, using non-dispersive infrared (CO , CO_2) and paramagnetic (O_2) analyzers.

2.2.3.5 Solid Combustion Products: Solid-Sampling Probe

In addition to being able to collect a solid sample that is representative of the material in the flame and to quench it at a sufficiently rapid rate, solid-sampling probes for use in flame research are subject to two requirements that prove to be very significant: (i) the probe must be large enough to contain both the water-cooling supply pipes and the facilities for collecting and handling the solid material, but, at the same time, (ii) the probe must be small so that its presence in the furnace has no significant influence on the flow conditions in the flame.

The standard procedure in the past was to construct the probe large enough to contain a filter chamber in the end that actually went into the flame. In such a probe, a suction line leads from outside the furnace to the filter chamber; another tube leads from the filter chamber to a nozzle that opens into the flame; a water jacket surrounds the whole system. When suction is applied to the end of the probe located outside the flame, hot material enters the nozzle and travels through the filter chamber where the solid material is collected. Heat is transferred from the sample to the cold walls of the tube leading to the filter chamber. This standard design necessitates an outer diameter of at least two inches and is, therefore, not practical in the present investigation; its use would obviously violate the second requirement mentioned above, namely, the presence of a cold, two-inch diameter probe would certainly exert a significant influence on the conditions in a flame that is only several inches thick itself.

In order to use a small diameter probe, a design was required in which the filter chamber is located outside the flame. The only parts of the probe that penetrate the flame are the nozzle through which the particles enter, the tube that leads from the nozzle to the filter chamber, and an appropriate water-cooled jacket. The lower limit for the size of this design was determined by the first requirement mentioned above, namely, sufficient space must be available in the probe to accommodate both the water-cooling features and the facilities for collecting and handling the solid sample. The facilities

for water-cooling are themselves subject to a serious lower limit in size because a certain minimum flow rate of cooling water is necessary to prevent thermal destruction of the probe and to insure adequate cooling of the sample. The size of the facilities for collecting and handling the solid material in the probe are also subject to a lower limit because of the following points that were learned by experience in the preliminary experiments. In the region of flames of pulverized bituminous coal that roughly corresponds to that of most rapid devolatilization, the particles become very sticky and tend to cling to the inside surface of the cold tube through which they are being transported; this tendency to stick to the tube promotes clogging and eventually leads to blockage of the passageway. The ability to resist clogging is inversely related to both the inside diameter of the sampling tube and the velocity with which the material is drawn through the tube. Therefore, in order to transport a sample of material from a point in the "sticky" zone of the flame to a filter chamber located outside the furnace, a probe must be used in which the diameter of the tube carrying the sample is above a certain lower limit. At the same time, the sampling tube must be below a certain upper limit because, with a given sampling velocity and probe temperature, the rate of cooling of the sample is inversely related to the inside diameter of the sampling tube.

After designing and testing several different models, each of which contributed something to the required knowledge about the critical dimensions and behavior of the probes, a design was finally attained which satisfied the above mentioned requirements (see Figure 11). The essence of this design is its ability to remove a sample from the flame, quench it rapidly, separate the solid from the gaseous material, and collect the solids for further study, all with only a small, 5/8 inch portion of the probe inside the flame. This probe is composed of three individual units, each of which is water-cooled, and which are easily disconnected to permit a thorough cleaning after the collection of each sample. The probe is of the suction type, with the sample being drawn through a filter chamber where the solid material is collected on a filter paper, the area of which is relatively large to avoid a large flow resistance. The filter paper used (Glass Fiber Type E - 2 in. diameter; Gelman Instrument Company) was designed to trap all particles greater than 3 microns, which at the same time permitting a large flow rate of gas through the unit. However, once the filter cake begins to form, particles as small as a fraction of a micron are trapped.

The nozzle is designed to offer the selection of a 90 degree entrance or a "straight-through" entrance, the particular entrance desired being chosen by eliminating its alternate with a brass plug. This feature was incorporated into the design at a time when clogging by sticky particles was thought to be promoted by forcing them to execute a 90 degree turn upon entering the probe. However, experimental tests disproved this hypothesis, and the preferred 90 degree entrance was used exclusively in collecting samples in the principal data runs. The 90 degree nozzle is preferable because it allows the entrance into the probe to be directed upwards when the probe is positioned horizontally. Since this is the same direction (but

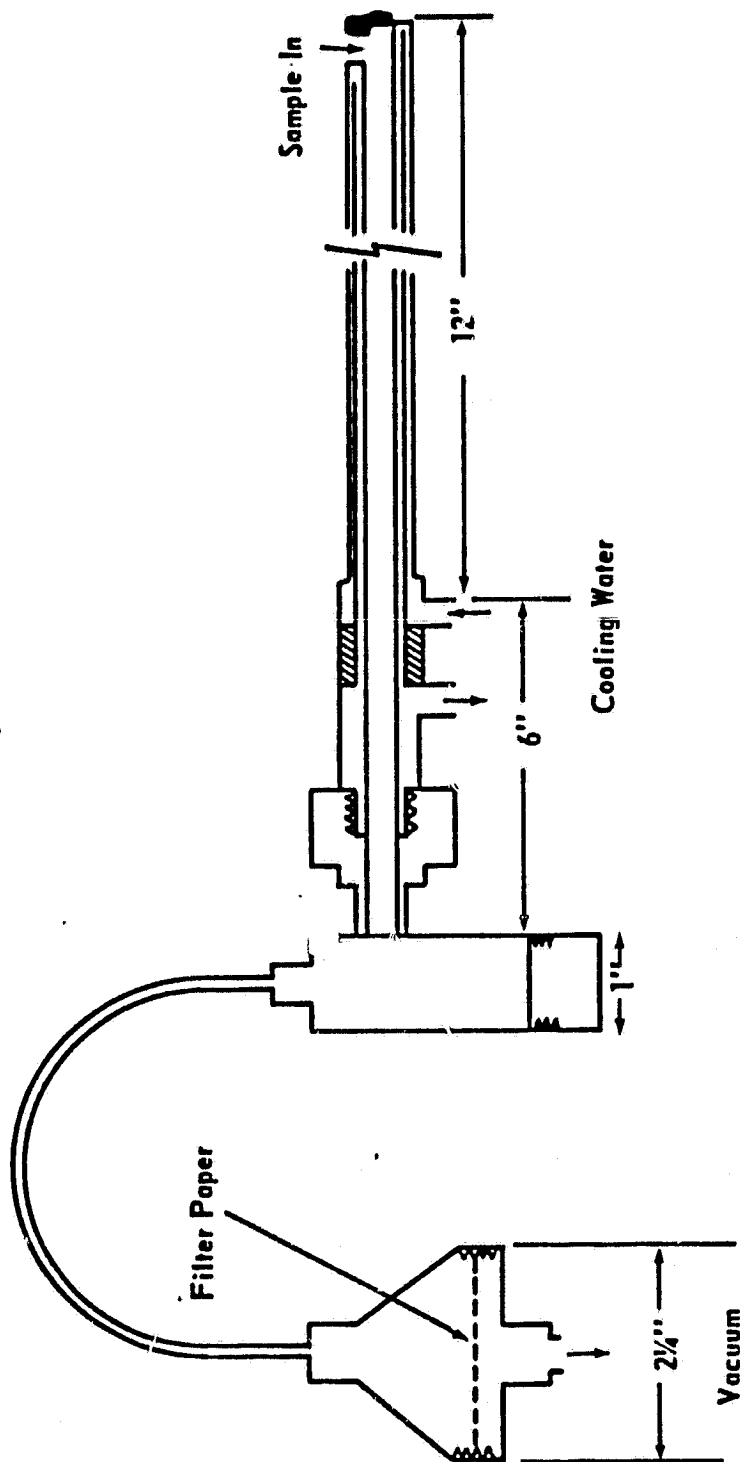


Figure 11. SOLID-SAMPLING PROBE

of opposite sign) as the movement of the particles in the flame, the particles can enter the probe without changing their direction until they are already inside the nozzle. With a correct suction velocity (which had to be determined in this investigation) such a nozzle is capable of collecting samples which are true representatives of the material in the flame.

The passageway through which the sample first flows is a standard 0.25 inch copper tube (0.315 in. I.D.). From the point of view of rapid quenching of the sample, a smaller tube would be more desirable; however, probes equipped with smaller tubes were designed, built, and thoroughly tested in preliminary experiments which showed that diameters smaller than the one finally used were not practical for use in this experiment because of blockage by sticky particles.

The second, longer section of the probe was designed to be able to permit particles to cling to the cold walls, without succumbing to blockage of the passageway or a significantly decreased rate of cooling. The cooling surfaces of this long annulus collect a very significant portion of the sample when probing the sticky region of the flame. This section of the probe finishes the cooling process which occurs mainly in the first section.

The size of the portion of the probe actually penetrating the flame (5/8 inches in diameter) is perhaps not as small as would be desired ideally for avoiding a significant effect on the conditions in the flame; but here again, this particular size was used out of necessity, since a significantly smaller tube would not contain both the tube through which the sample flows and the inlet and outlet passageways for cooling water. However, this size was regarded as suitable with respect to not affecting the flame since, in a special experiment, it was found that no significant change occurs in the temperature of the inside surface of the combustion chamber at a given point when the probe is injected into the center of the flame at the same location.

2.2.4 Combustion Data Acquisition

The plane flame furnace was fired at 8-10 pounds of pulverized JPL coal per hour and at +20% excess air. In order to better simulate the pulverized coal characteristics used in typical electric utility power boilers, for which the JPL-desulfurized coal is ultimately intended, the JPL-supplied coals were pulverized to a mass mean particle diameter 75 microns. This procedure also permits any necessary comparisons to be made between the JPL coals and other solid fuels test-burned using the PSU-FCL plane flame furnace.

Flame and wall temperatures and compositions of gaseous and solid products of combustion were characterized as a function of residence time (axial distance down the furnace centerline) by sampling the combustion environment through ports distributed along the vertical axis of the furnace (see Figure 1). Residence time was calculated as a function of downward distance with the use of the coal/air cold volumetric flow rate, the square-cross-sectional area of the combustion chamber, and the flame temperature profile. The volumetric flow rate (cm^3/sec) divided by the cross-sectional area (cm^2) yields a flow velocity (cm/sec). The ratio of the flame to the ambient temperature times the input cold flow velocity yields the flame speed (cm/sec). The downward integrated position or flame thickness (cm) divided by the flame speed (cm/sec) at that point yields the elapsed residence time from time zero to that position (sec). Once the furnace has been calibrated in terms of residence time, then ignition times, burning velocities, and burnout times were determined as a function JPL-coal sample. These data indicate how well JPL-desulfurized coals will perform as boiler fuels on a comparative basis.

The progress of combustion in a pulverized coal flame is best monitored by measuring the appearance of carbon dioxide products and/or the disappearance of elemental carbon in the fuel, and thus following "carbon burnoff." Carbon burnoff can be measured in two independent ways: (a) on a gas-phase product of combustion basis (CO_2) from fuel ultimate analysis information and (b) on a solid-phase product of combustion basis (elemental carbon in the char) from fuel ultimate analysis information. From the coal's ultimate analysis, one can readily calculate [2] the identities and quantities of gaseous products of combustion at 100% carbon conversion and at any stoichiometry. The percent CO_2 in the exhaust gases at complete combustion and at +20% excess air was calculated for each JPL-coal. The ratio of the experimentally measured CO_2 flame concentration and this absolute CO_2 maximum concentration at any downward vertical position within the furnace yields the extent of combustion up to that particular residence time. These data can be independently checked by collecting a solid sample and measuring its elemental-carbon content. By comparing this information with the elemental-carbon content in the unburned-coal's ultimate analysis, one can again measure the progress of carbon burnout as a function of residence time. In this calculation, it must be assumed that all the elemental carbon is converted to CO_2 . Independent measurements have validated this assumption in

air-rich (+20% excess air) flames, i.e., there was no carbon monoxide or hydrocarbons in the exhaust gases and the exhaust O_2 concentration was a constant 3.5%. With these data on carbon burnoff and residence time, important events in the initiation, propagation, and termination of a flame can be defined: ignition time, burnout velocity, and burnout time, respectively. Ignition time is defined as the residence time required for 1% coal carbon burnoff. Burnout time is the time required for 100% carbon burnoff. The burning velocity is the quotient of the distance over which a flame exists (or flame thickness) and the residence time that has transpired over that interval. Burning velocity can be thought of as an overall rate of combustion once a flame has been ignited.

2.3 RESULTS AND PROGRESS MADE ON CONTRACT TASKS

2.3.1 Test Coal Shipments and Analysis

All nine JPL-desulfurized and supplied coals have been test-burned in the plane flame furnace at this time. As per the Statement of Work, ignition times, burning velocities, and burnout times have been determined for each JPL coal sample.

The JPL shipped the test coal samples to the PSU-FCL in three stages. On December 17, 1981, the PSU-FCL received 30 pounds each of the three (3) raw coals, with identities given according to the PSU Coal Research Section Coal Sample and Data Bank, PSOC-282, -276, and -230. On February 5, 1982, the PSU-FCL received 17 pounds each of the JPL-chlorinated (CL) and mildly-desulfurized versions of the aforementioned parent coals. On March 10, 1982, the PSU-FCL received the final shipment of 18 + 1 pounds each of the JPL-chlorinated/hydrodesulfurized (CL/HDS) and severely-desulfurized coals.

The coal characteristics of all nine JPL-test coals are given in Table I. Each has been assigned a test number according to convention at the PSU-FCL. Compositional data on the three raw coals was taken from JPL Publication 81-82 [1]. The compositional data on the JPL-treated coals were communicated to Prof. Reuther in a letter from Dr. Kalvinskis dated April 9, 1982 (JK-dy-TRSE-345-4). This communication makes up Appendix III.

TABLE I
COMPOSITIONS OF RAW AND JPL-DESULFURIZED COALS

PSU-FCL- Test No.	Coal	JPL Process	Ultimate Analysis					Proximate Analysis					Heating Value (Btu/lb)
			C	H	N	S	O	Ash	(dry, wt%)			Moisture (%)	
									Volatile Matter	Fixed Carbon			
(dry, wt%)													
JPL-1	PSOC-282	RAW	74.8	4.82	1.69	1.60	9.92	6.70	33.80	59.5	3.10	13,092	
JPL-2	PSOC-282	CL	77.2	3.92	1.83	0.68	5.70	7.76	45.10	67.2	0.71	13,060	
JPL-3	PSOC-282	CL/HDS	82.0	2.13	1.75	0.32	2.12	10.10	7.57	82.3	1.18	13,167	
JPL-4	PSOC-276	RAW	71.6	5.67	1.28	3.91	5.87	11.50	37.20	51.3	1.89	12,755	
JPL-5	PSOC-276	CL	72.7	3.93	1.46	1.31	9.67	9.88	23.50	66.6	0.48	12,792	
JPL-6	PSOC-276	CL/HDS	84.4	2.07	1.73	0.53	2.14	8.63	6.50	84.9	0.82	13,479	
JPL-7	PSOC-230	RAW	69.6	4.40	1.06	0.87	14.9	9.03	38.90	52.1	7.26	11,892	
JPL-8	PSOC-230	CL	77.1	4.14	1.11	0.62	6.53	9.79	34.20	56.0	0.61	12,127	
JPL-9	PSOC-320	CL/HDS	80.9	2.14	1.20	0.38	2.82	12.00	6.25	81.8	0.82	12,524	

2.3.2 Combustion Test Results on JPL-Coals

2.3.2.1 Plane Flame Furnace Standard Conditions

Prior to a combustion test on any JPL-desulfurized coal or parent coal, the plane flame furnace was preheated to a set temperature using a standardized ignition procedure. Previously, experiments had been executed to calibrate the plane flame furnace according to its time/temperature preheat history. Figure 12 shows the highest-temperature regions of the plane flame furnace combustor profile as a function of preheat time. Thermocouple stations #10-12, at 30-76 centimeters downward from the water-tube bank, recorded the three highest wall temperatures within the combustor temperature profile when the plane flame furnace was preheated with a natural gas flame; station #11 typically recorded the highest furnace wall temperature. Hence, in order to experimentally set the preheat temperature of the plane flame furnace at, e.g., 500°C, 700°C, or 900°C, the natural gas flame was fired for 0.5, 1.0, or 7.0 hours, respectively. Once the desired preheat temperature was reached, the gas burner was shut off, removed, its entry port plugged, and the desired steady-state pulverized coal feed established. The coal firing rate was set at 10^4 Btu/hour corresponding to ca., 7.8 pounds of coal per hour; the coal/air stoichiometry was set at +20% excess air.

For all the combustion tests on JPL-coals reported in this document, furnace preheat was constant at 900°C.

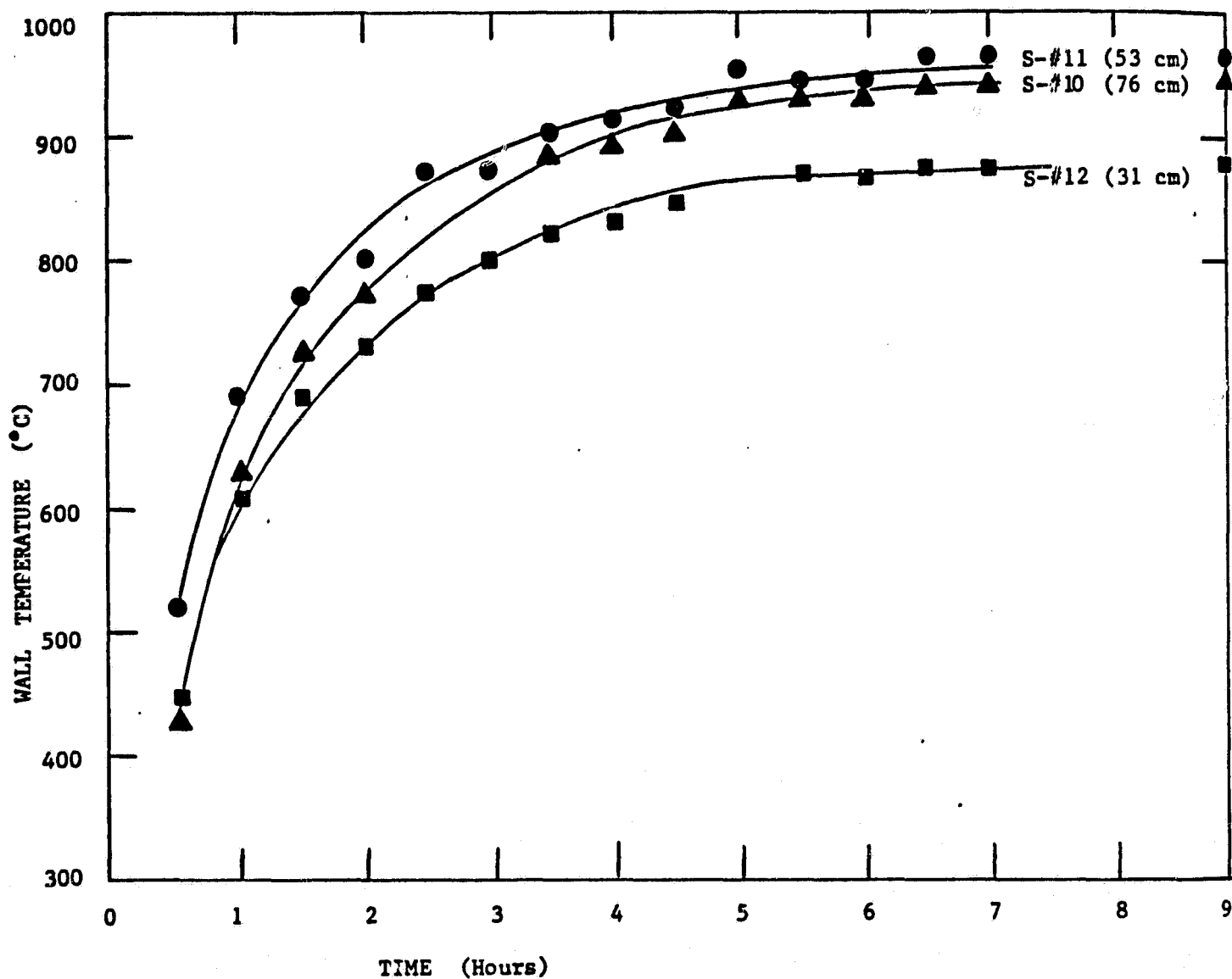


Figure 12. Variation of maximum furnace wall temperature at specific locations downstream of the tube bank as a function of time for natural gas/air flames.

2.3.2.2 Gas-Phase JPL-Coal Flame Graphical Data

Figures 13-15 graphically present the plane flame furnace exhaust carbon dioxide (CO_2) profiles for each of the three JPL-coal shipments, i.e., sample Nos. JPL-1, 4, 7 (Fig. 13); JPL-2, 5, 8 (Fig. 14), or JPL-3, 6, 9 (Fig. 15). In these figures, each of the 3 raw, chlorinated, or chlorinated/hydrodesulfurized coals are compared with the same process condition (or none) for the three different coals. The CO_2 profile data given in Figs. 13-15 have been reported as a function of residence time. It should be noted that the flame temperature profiles for all three sets of three samples were spacially and quantitatively comparable to each other. Specifically, the wall temperature profiles for all nine JPL-coal flames peaked at a temperature of $1350 \pm 40^\circ\text{K}$ and at a residence time that was ca. 100 ± 25 milliseconds (msec) prior to the residence time at which the maximum in the CO_2 exhaust gas concentration was realized. The flame cooling rates after their respective maxima were also comparable. A succinct way of summarizing and interpreting this JPL-coal flame temperature profile behavior is to state that once ignited, JPL-desulfurization had little or no effect on the maximum temperature of the raw coal and that the delay in reaching these maxima was as one switches from raw-to-chlorinated-to-chlorinated/hydrodesulfurized coal reflects only the difficulty in ignition.

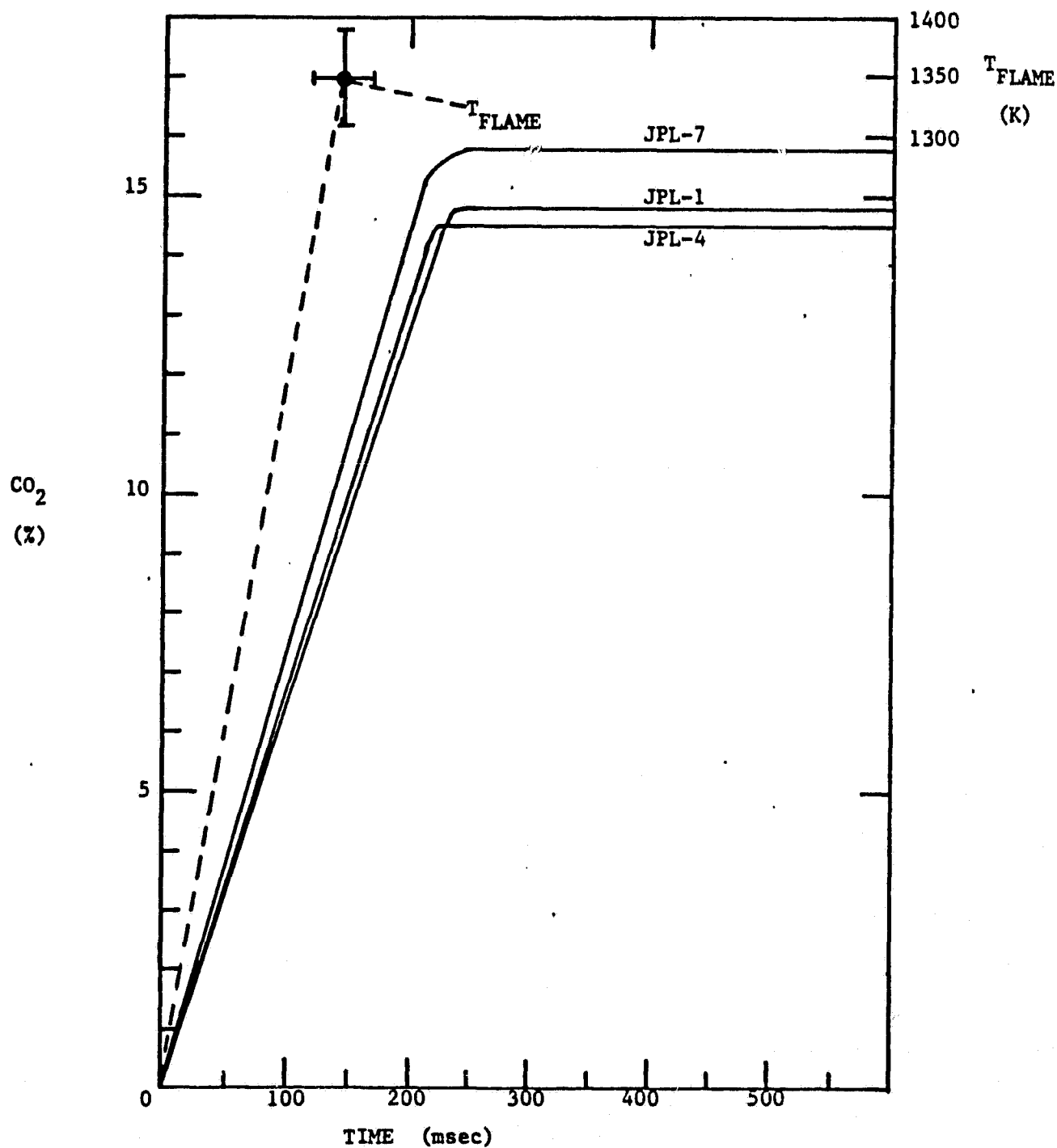


Figure 13. Gas-phase combustion performance characteristics of raw JPL-test coals: JPL-1, JPL-4, JPL-7.

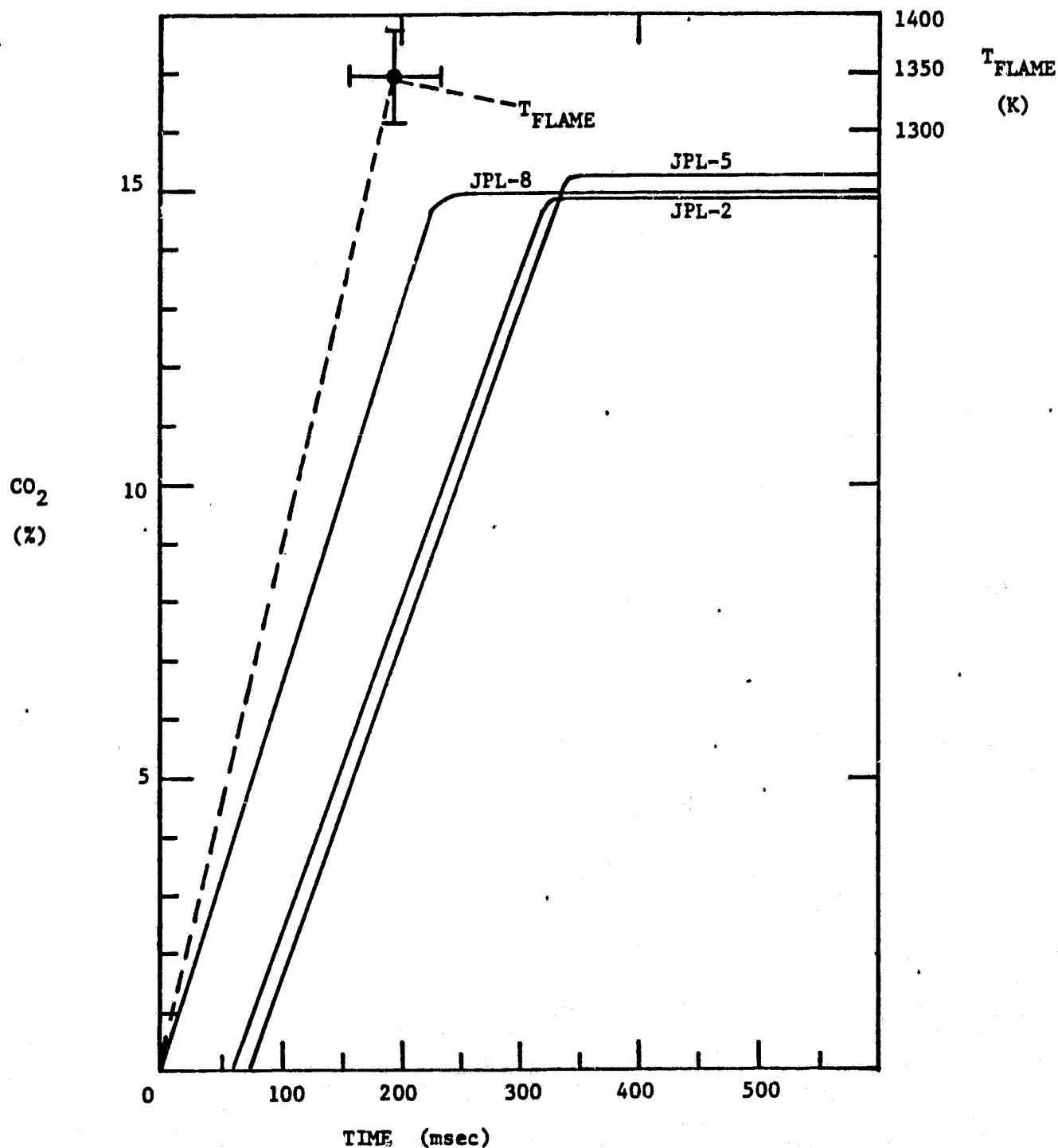


Figure 14. Gas-phase combustion performance characteristics of chlorinated JPL-test coals: JPL-2, JPL-5, JPL-8.

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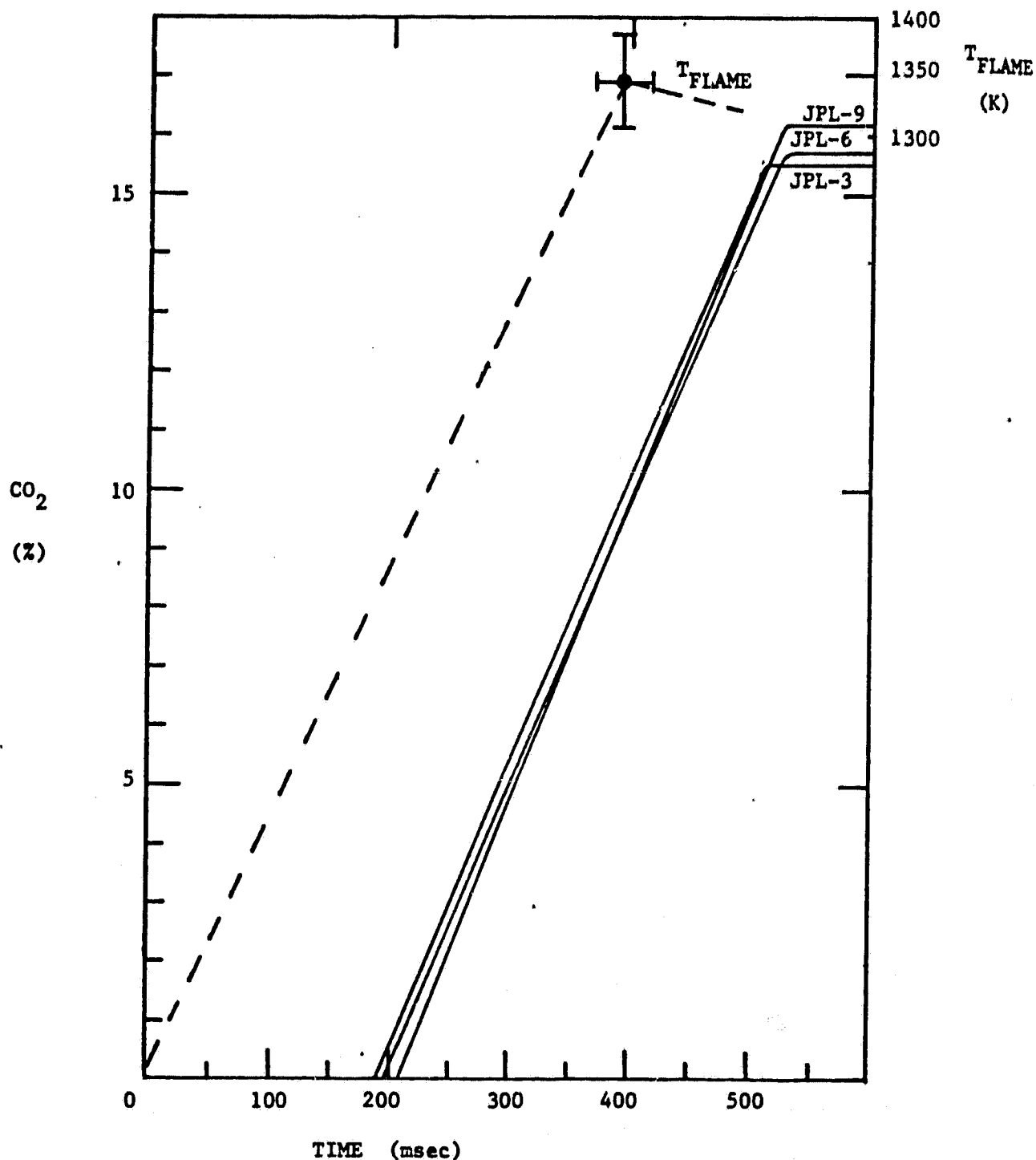


Figure 15. Gas-phase combustion performance characteristics of chlorinated/hydrodesulfurized JPL-test coals: JPL-3, JPL-6, JPL-9.

Figures 16-18 present the same plane flame furnace CO₂ profile data as given in Figs. 13-15, but now they are plotted so that the effect of chlorinolysis and chlorinolysis/hydrosulfurization on the (ignition, reaction, and burnout) combustibility of each different raw coal is illustrated. The trends in the results as a coal is desulfurized (and devolatilized) were not unexpected: ignition time is delayed, burning velocity or overall rate of reaction decreased, and burnout time was prolonged. The raw coals, JPL-1, 4, and 7, all exhibited a zero ignition delay time. As each raw coal was desulfurized, with the exception of JPL-8 -- which was not desulfurized and devolatilized to the same extent that its analogues (JPL-2 and 5) were -- the JPL-processed coal derivative exhibited an ignition delay time.

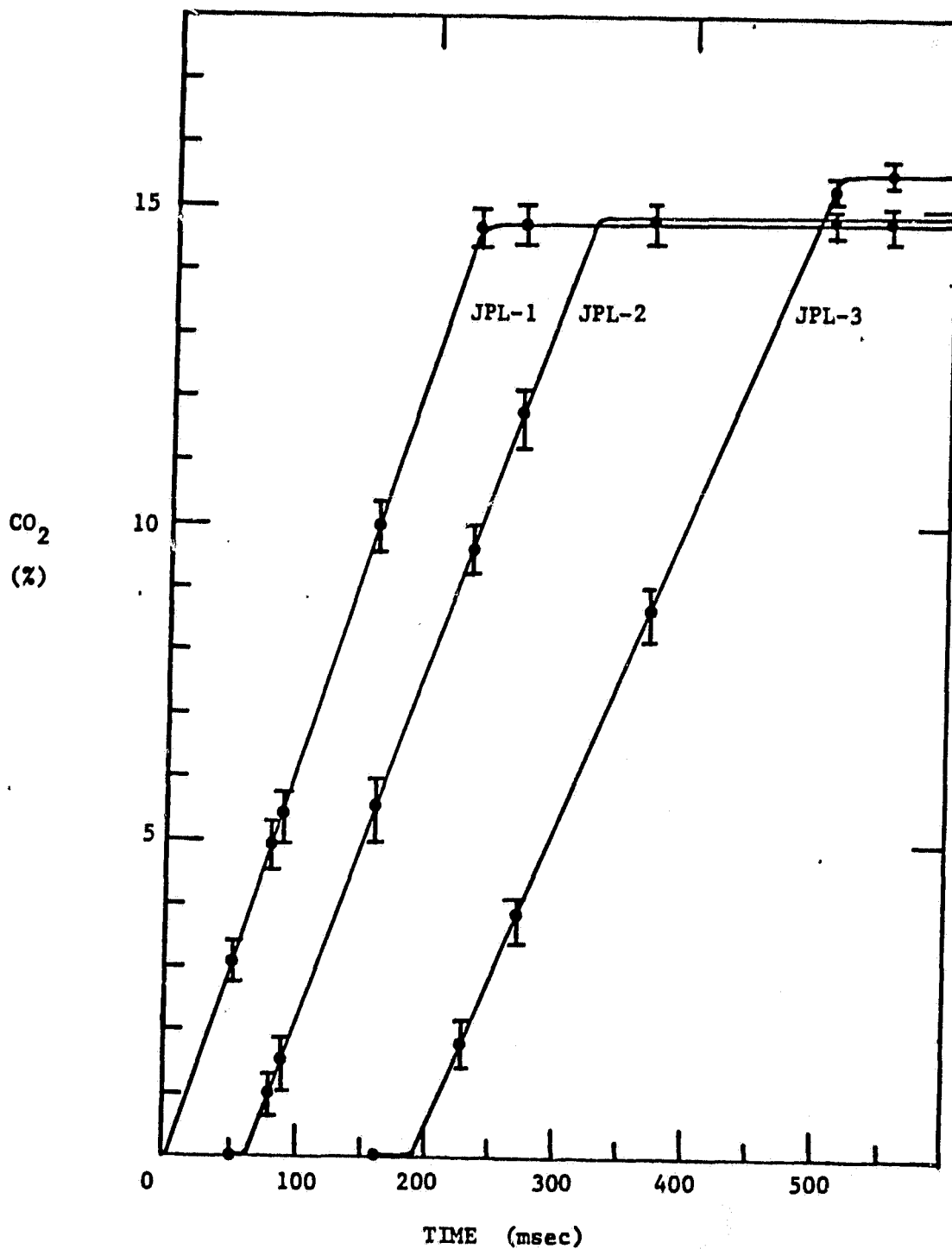


Figure 16. Gas-phase combustion performance characteristics of raw and JPL-desulfurized PSOC-282 coal: JPL-1, JPL-2, JPL-3.

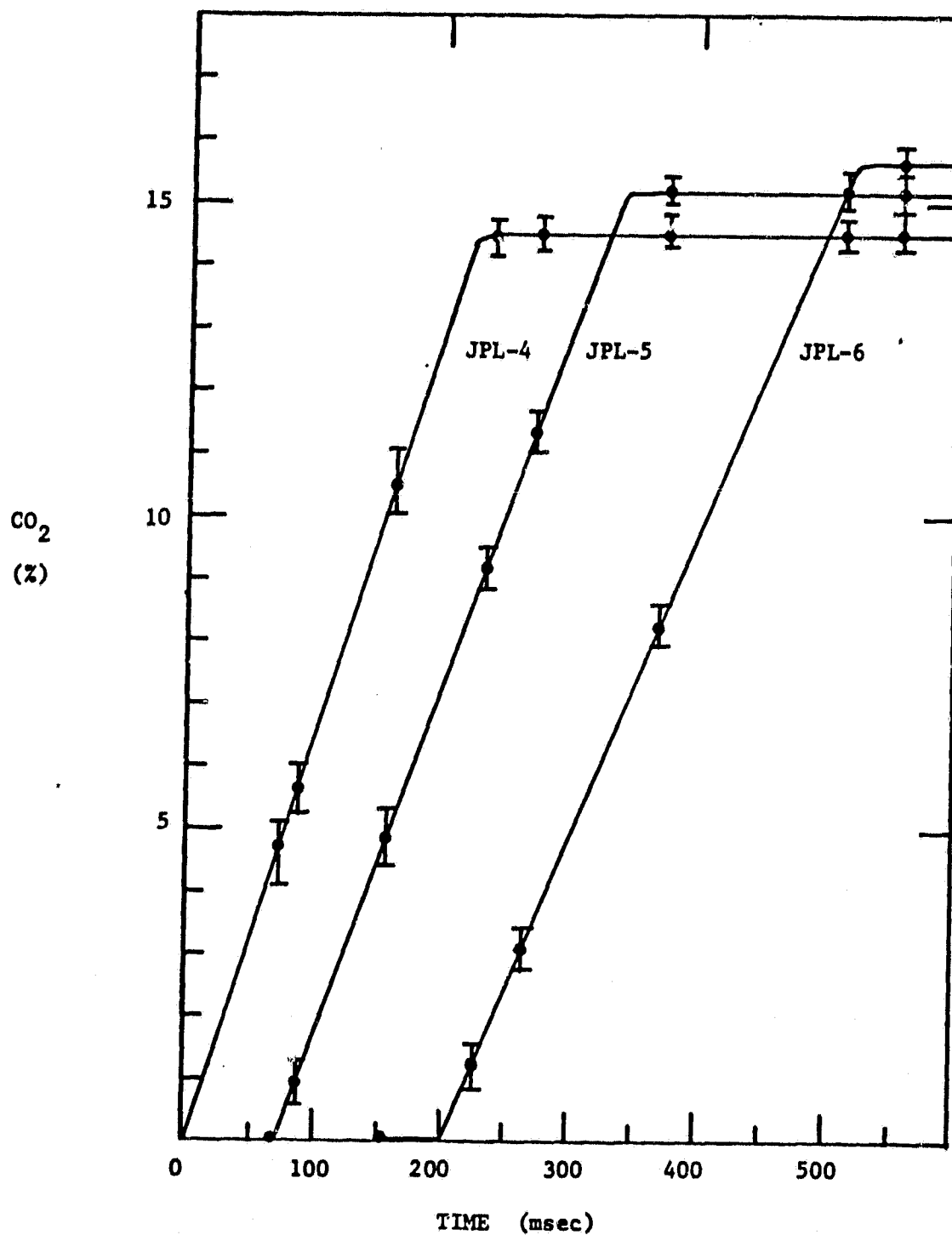


Figure 17. Gas-phase combustion performance characteristics of raw and JPL-desulfurized PSOC-276 coal: JPL-4, JPL-5, JPL-6.

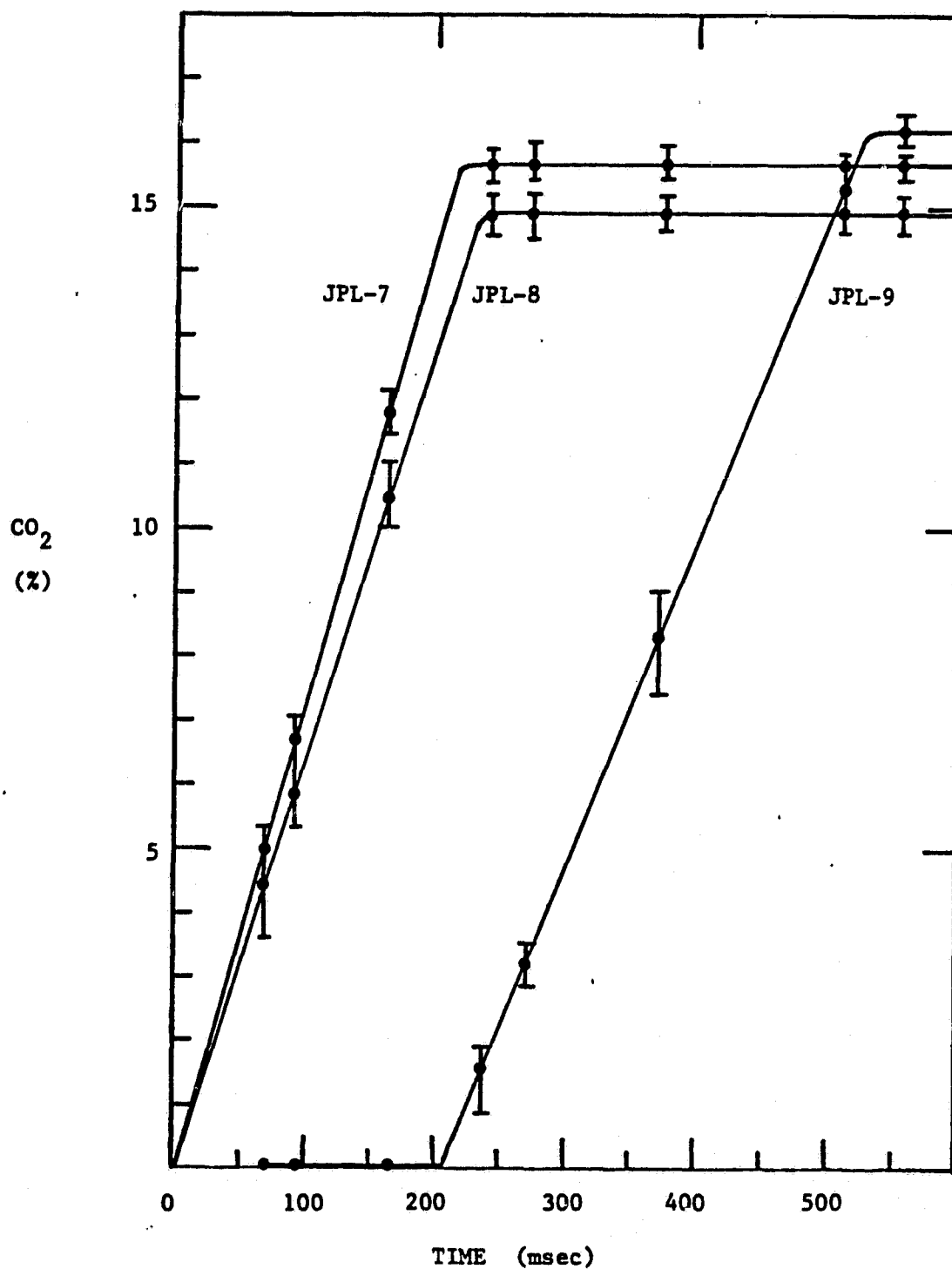


Figure 18. Gas-phase combustion performance characteristics of raw and JPL-desulfurized PSOC-230 coal: JPL-7, JPL-8, JPL-9.

2.3.2.3 Solid-Phase JPL-Coal Flame Graphical Data

In order to corroborate the gas-phase flame data concerning the progress of combustion, samples of the solid products of combustion (chars and, eventually, ash) were taken as a function of residence time within the furnace. The analytical work done on these samples was performed by The Pennsylvania State University Mineral Constitution Laboratory using a Carlo-Erba Elemental Analyzer #1106 for C-H-O-N determinations. Figures 19-21 illustrate the results of JPL-coal flame solid sampling in the same format as that given in Figs. 16-18, i.e., the effect of chlorinolysis and chlorinolysis/hydrodesulfurization on the combustibility of each different raw coal is illustrated.

The solid-phase JPL-coal flame data agreed very well with the gas-phase JPL coal flame data.

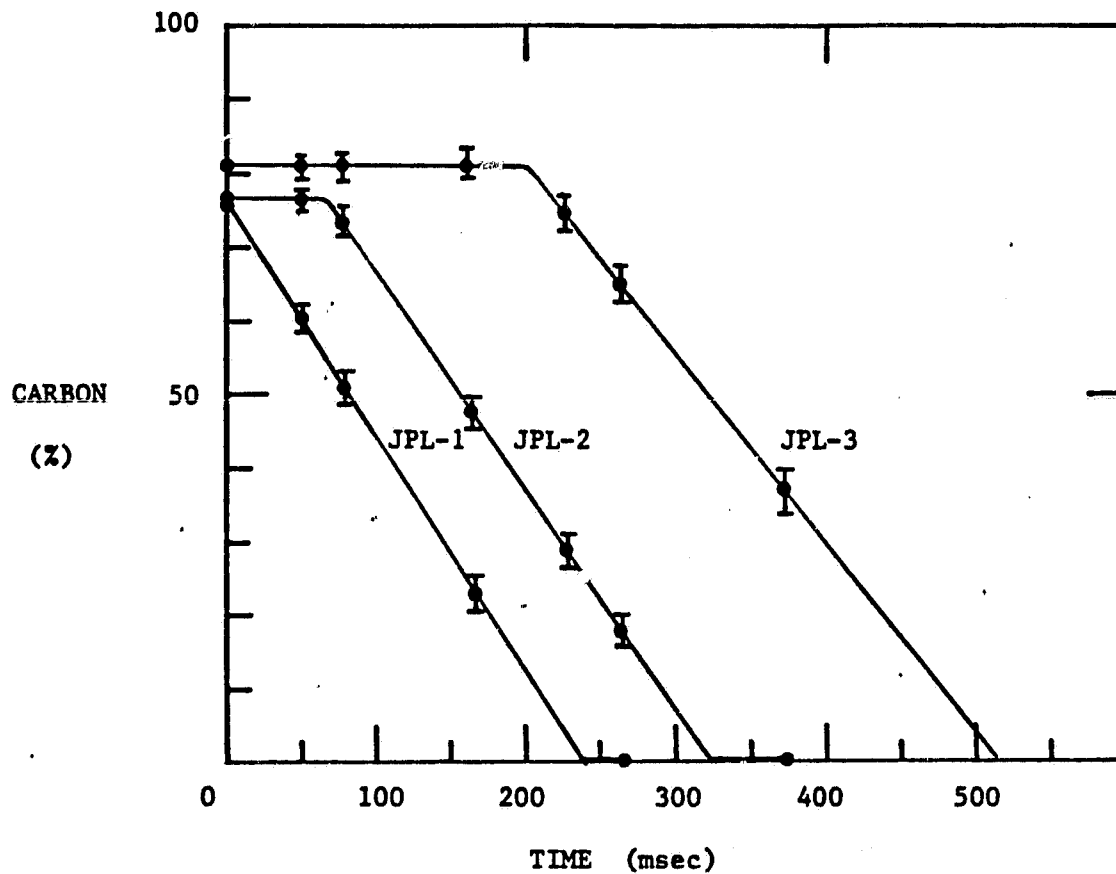


Figure 19. Solid-phase combustion performance characteristics of raw and JPL-desulfurized PSOC-282 coal: JPL-1, JPL-2, JPL-3.

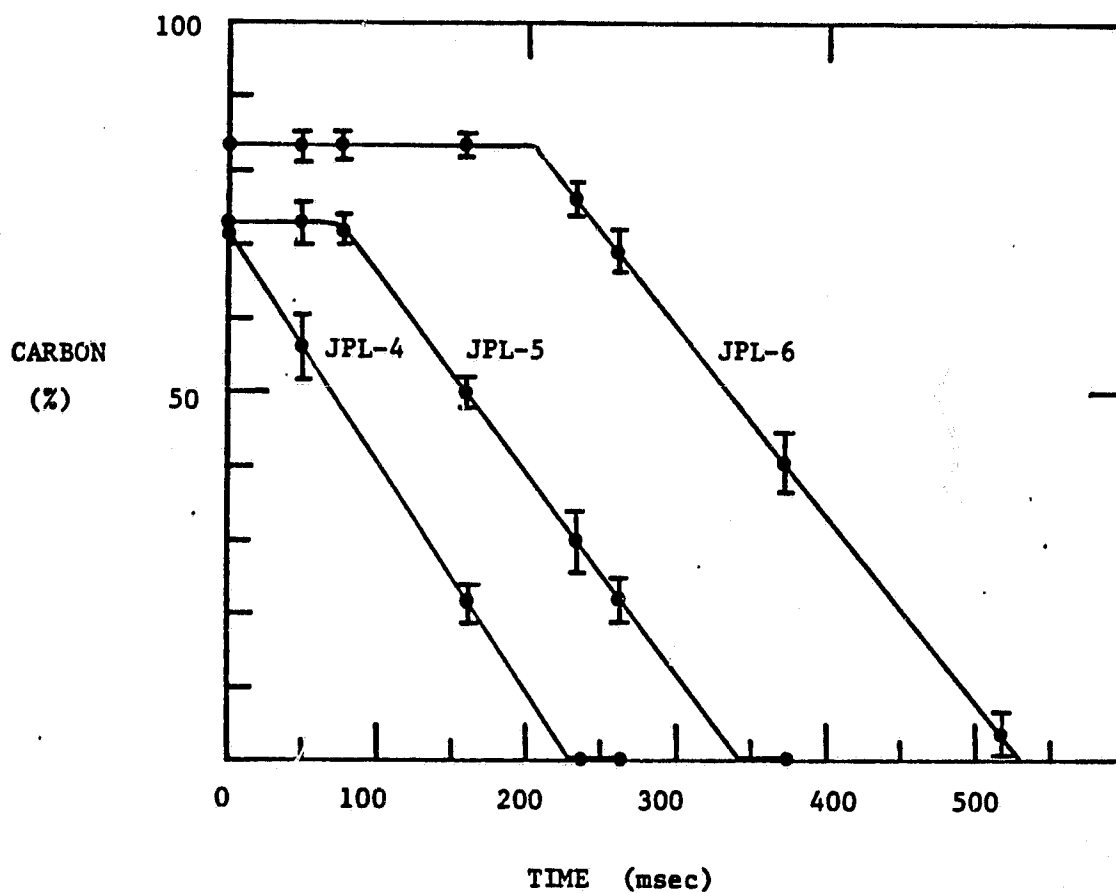


Figure 20. Solid-phase combustion performance characteristics of raw and JPL-desulfurized PSOC-276 coal: JPL-4, JPL-5, JPL-6.

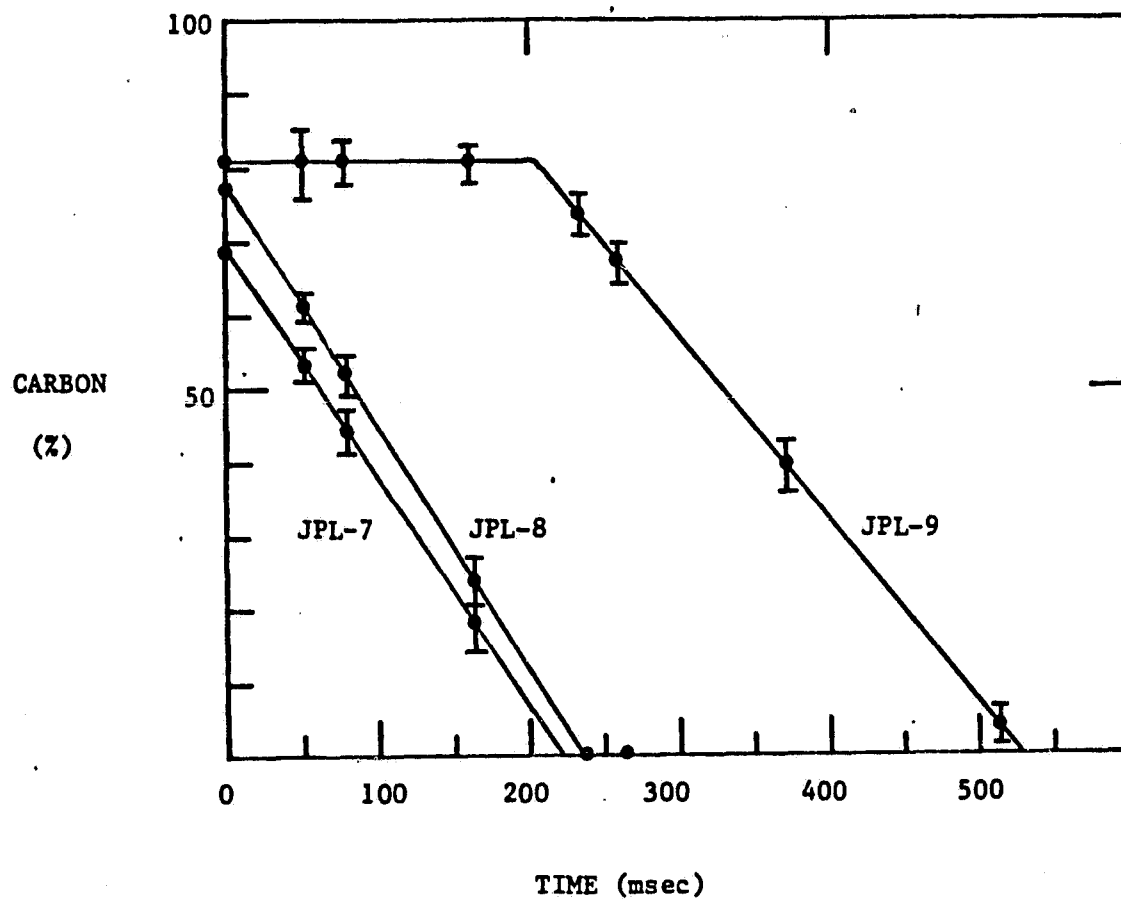


Figure 21. Solid-phase combustion performance characteristics of raw and JPL-desulfurized PSOC-230 coal: JPL-7, JPL-8, JPL-9.

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2.4. SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

All the data presented graphically thus far in Figs. 13-21 were numerically evaluated with the use of an Apple II microprocessor system in which are encoded equations that allow the quantification of the ignition, reaction, and burnout combustibility criteria defined in Section 2.2.4. This computer analysis produced the contract-required data, and more, which have been listed in Table II. The volatile matter contents of the nine JPL-test coals correlate well with their respective combustion performance characteristics, as expected; this is why the volatile matter content of each coal is listed in Table II. Also included in Table II, is the SO₂ pollutant emission potential for each JPL-test coal assuming 100% conversion of fuel-bound-sulfur to SO₂. These data will be used in the discussion of tradeoffs between loss of combustibility and desulfurization upon JPL chlorinolysis/hydrodesulfurization.

These singular combustibility data as generated by the FSU-FCL plane flame furnace allows one to decouple the flame initiation, propagation, and termination events from each other in order to identify which is primarily responsible for the loss of combustibility upon JPL-coal processing. Table II quantifies the following generic behavior in terms of fuel combustibility: as the volatile matter content decreases upon JPL-desulfurization, the respective raw coal's ignition time is delayed by a factor of 70, its burning velocity or overall reaction rate is retarded by a factor of 1.5, and its burnout time is prolonged by a factor of 1.4. These data clearly indicate that of the three events, ignition, reaction, and burnout, whose total represents the total flame residence time, ignition dominates. On average, for the 3 parent coals listed, decreasing the raw coal volatile matter content by 80% (from 36.6 to 6.8%) via JPL-chlorinolysis/hydrodesulfurization, results in a generic two-fold-plus increase (230 to 530 msec) in total flame residence time. Of the average 300 msec generic increase in the total flame residence time as the raw coal is generically desulfurized and devolatilized by about 75% and 80%, respectively, approximately 68% is directly attributable to the loss of ignition quality, i.e., a rather long ignition delay time (on average, ca. 200 msec) develops when there was none for the raw coal.

The remainder of the increase in total flame residence time upon severe JPL-desulfurization (ca. 100 msec) is attributable to the retardation of the raw coals overall reaction rate once ignited, as is reflected in the burning velocity data and is quantified in the burnout time data. On average, for the concomitant severe desulfurization and devolatilization of the raw coal, the burnout time increases from 230 to 324 msec. The retardation of raw coal burning velocities and lengthening of burnout times is probably the consequence of coal pore structural changes and fixed-carbon increases occurring upon JPL chlorination/hydrodesulfurization.

Before discussing recommendations for alleviating the aforementioned ignition and burnout problems, that seemingly will unavoidably occur upon JPL-coal desulfurization, one JPL test coal, JPL-8, must be

TABLE II

COMBUSTIBILITY DATA ON RAW AND JPL-DESULFURIZED COALS

PSU-FCL- Test No.	Coal	JPL Process	Volatile Matter (%)	Ignition Time (msec)	Ignition Delay Time (msec)	Burning Velocity (cm/sec)	Flame Length (cm)	Burnout Time (msec)	Total Flame Residence Time (msec)	SO ₂ Pollution (lb/10 ⁶ Btu)
JPL-1	PSOC-282	RAW	33.8	0		31.3	40.3	239	239	2.44
JPL-2	PSOC-282	CL	25.10	61		28.1	44.8	266	327	1.04
JPL-3	PSOC-282	CL/HDS	7.57	198		23.2	54.3	322	520	0.49
JPL-4	PSOC-276	RAW	37.20	0		32.8	38.4	228	228	6.13
JPL-5	PSOC-276	CL	23.50	73		27.5	45.8	272	345	2.04
JPL-6	PSOC-276	CL/HDS	6.50	206		23.0	54.8	325	531	0.79
JPL-7	PSOC-230	RAW	38.90	0		33.7	37.4	222	222	1.46
JPL-8	PSOC-230	CL	34.20	0		31.6	39.9	237	237	1.03
JPL-9	PSOC-230	CL/HDS	6.25	208		22.9	54.9	326	534	0.61

singled-out for comment. The raw test coal (PSOC-230) of this series of fuels (see Table II), ignites without an ignition delay and burns out without difficulty. It cannot be directly fired in a coal combustor without the employment of SO₂ emission control technology because it does not meet the Environmental Protection Agency (EPA) upper SO₂ emission limit of 1.2 pounds per million Btu fired (see right-most column of Table II). Upon mild JPL-desulfurization via chlorinolysis, JPL-8 becomes an SO₂ compliance coal. More important is the fact that this sulfur cleanup is accomplished with only a minimum alteration of PSOC-230 combustibility, i.e., it did not result in the appearance of an ignition delay time and it only causes a 7% increase in burnout time. Hence, JPL-chlorinated PSOC-230 could indeed be thought of as a premium fuel.

With this SO₂-removal/loss of ignition-theme in mind, it is informative to ask the following question: what would the loss-of-ignition penalty from the loss-of-volatile matter content be for the other two raw coals, PSOC-282 and PSOC-276, for them to come into SO₂-compliance as the direct result of JPL chlorinolysis or chlorinolysis plus hydrodesulfurization? Figure 22 has been prepared to help answer this question. In Figure 22, PSU-FCL-measured ignition delay time data and calculated maximum SO₂ emission data are plotted as a function of volatile matter content for all three types of raw coals. Also drawn in Figure 22 is the EPA upper emission limit for SO₂. As should be obvious, the ignition delay time correlates linearly very well (95+% coefficient) with volatile matter. A best straight line has thus been drawn through the ignition delay time data as a function of volatile matter content. Smooth curves have been drawn through the SO₂ emission data as a function of volatile matter to find the point at which they intersect the EPA SO₂ upper emission limit. As already discussed, mildly desulfurized PSOC-230 raw coal complies with the SO₂ limit and is readily ignitable, the latter because its volatile matter content remains high. For PSOC-282 raw coal, compliance desulfurization via the JPL process would require the reduction of its volatile matter content to about 26.8% (from 33.8%). This loss-of-volatile matter content upon SO₂ compliance would result in an ignition delay penalty of only 50 msec. For PSOC-276 coal to become an SO₂ compliance coal via JPL treatment, it would have its volatile matter content reduced drastically, from 37.2% to 16%. This would result in an ignition time delay penalty of about 130 msec.

How can these results be best interpreted? From his decade of experience in combustion research, Prof. Reuther is aware of an industrial "rule of thumb" that states that utilities typically think coals having a volatile matter content of 20% or greater will offer no combustibility problems, whereas those having less than 20% may very well be troublesome. The last determination in this report on the loss of volatile matter content-loss of ignition tradeoff upon JPL-desulfurization produces a very encouraging result, from JPL's viewpoint: the JPL-chlorinolysis and/or hydrodesulfurization process is a promising means for producing SO₂-compliance coals from high-sulfur PSOC-282 and 276 coal feedstocks that will either surpass

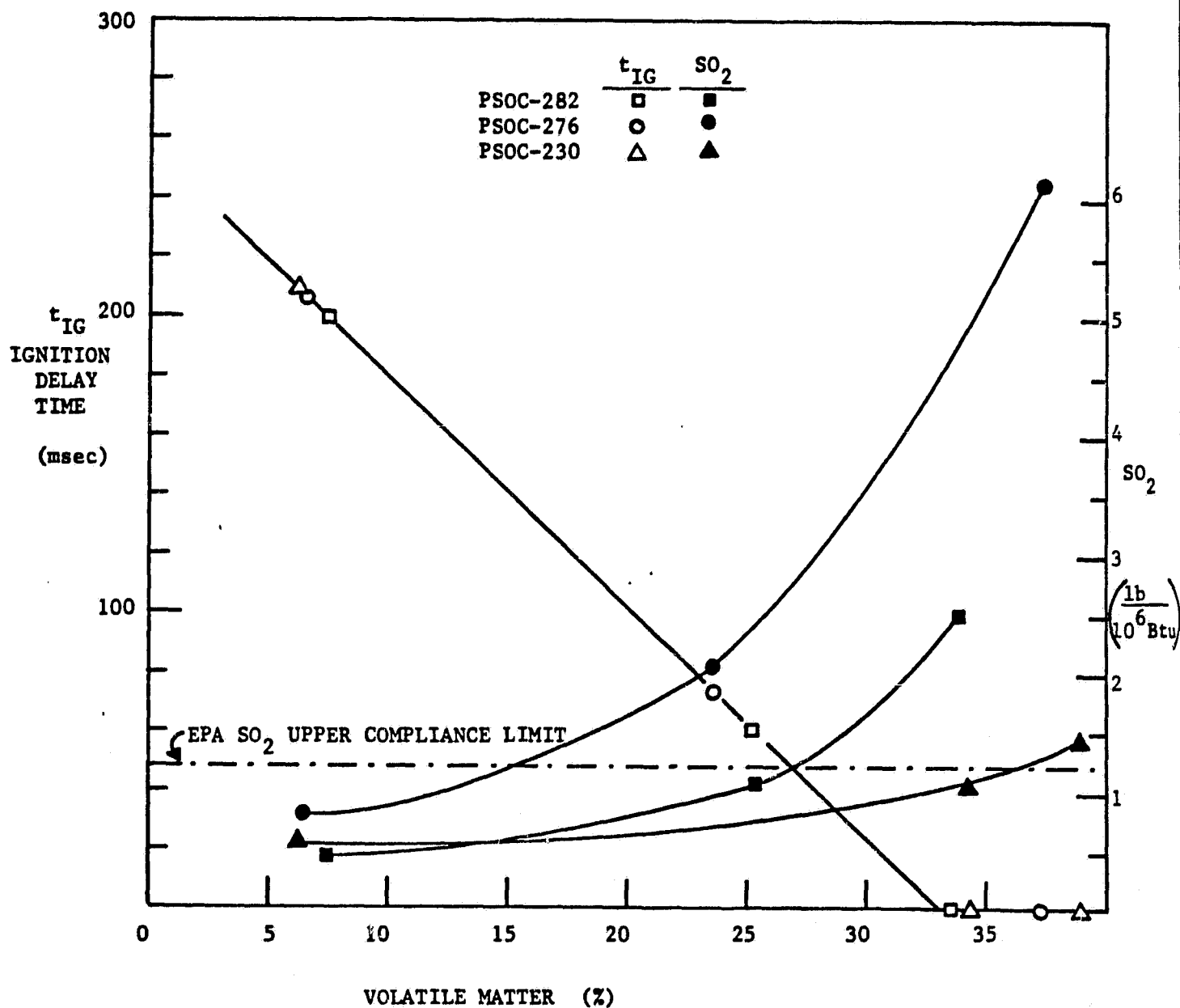


Figure 22. Trade-off between sulfur removal and ignition performance upon JPL-desulfurization as a function of coal volatile matter content.

or nearly-miss the coal combustion industries cutoff limit for acceptable combustibility.

In summary, the latter analysis of the plane flame furnace combustibility data on JPL-desulfurized coals seems to indicate that in two cases out of three (PSOC-282 and 230), the JPL desulfurization process produces a coal that is both clean (in terms of SO₂ pollution) and easy (in terms of ignitibility) to burn.

SO₂

The discussion thus far has primarily focused on stopping the JPL desulfurization process at the SO₂ compliance limit. One must ask if one would even contemplate using the severely JPL-processed coals, given their somewhat inferior combustibility characteristics. This question actually reduces to one that asks if these severely desulfurized, very low volatile JPL-process coals could be burned in a utility boiler. The Principal Investigator's answer to this question is an rather optimistic yes, and so for two reasons. The first has to do with the fact that the low-sulfur, low-volatile, severely JPL-processed coals need not be directly burned neatly. In other words, the very-low sulfur JPL-processed coals could be blended with higher-sulfur coals to produce a coal that simultaneously meets the utility industry's combustibility criteria and EPA's SO₂ pollution limit. Gogot and Hensel of Combustion Engineering, a major utility boiler manufacturer, have carefully considered the concept of blending coals to meet SO₂ emission standards [3]. Prof. Reuther suggests that if an easy, but dirty to burn raw (high volatile, high sulfur) coal were blended with a difficult, but clean to burn (low volatile, low-sulfur) JPL-desulfurized coal, the coal-fired utility boiler industry would have a premium, easy and clean to burn coal and the JPL would have a promising market for its chlorinolysis/hydro-desulfurization process.

1b
0.6 Btu

Secondly, Prof. Reuther has asked the question of whether or not burner technology exists to help to circumvent the ignition delay problem for the severely desulfurized coals. One finds the answer to this question in the combustion research literature that concerns directly-firing pulverized anthracite coal, a natural low-sulfur, low-volatile solid fuel [4-6]. The universal finding of these programs indicated that long ignition delay times could be shortened by enhancing recirculation of hot combustion gases near the pulverized anthracite burner [3,4] and that sluggish flame velocities could be accelerated by increasing the fineness of the pulverized fuel grind [3]. Moreover, judicious selection of flame-furnace configuration, especially, that involving vertical-firing, is another means by which to acceptably ignite and burnout low-volatile fuels (6), such as those with less than 15% volatile matter. Down-fired coal combustors could now, in principal, successfully fire low-volatile severely JPL-desulfurized coals. It would be useful to learn how many of these down-fired units are currently in operation.

In conclusion, the PSU-FCL plane flame furnace combustion tests on JPL-desulfurized coals indicate that although the combustibility characteristics of high-volatile/high sulfur coals are diminished

upon JPL desulfurization, their average extent is one that should not be thought of as prohibiting JPL-process coal from direct use in utility boilers. It is the expert opinion of the Principal Investigator that the JPL desulfurization process appears to offer promise and competitiveness with other SO₂ control strategies, such as flue gas desulfurization, fluidized bed combustion, coal conversion, and mechanical beneficiation [7], and research and development concerning it should be actively continued.

James J. Reuther 15 MAY 82

Dr. James J. Reuther
Assistant Professor of Fuel Science
Principal Investigator
JPL Contract 956123

2.5 REFERENCES

1. Kalvinskas, J., Rohatgi, N., and Ernest, J.: Final Report: Coal Desulfurization by Low Temperature Chlorinolysis, Phase III, JPL Publication 81-82, March 1, 1981.
2. Davies, C.: "Combustion Calculations," Chap. 2, pp. 25-66, Calculations in Furnace Technology (Pergamon Press, New York, 1966).
3. Bogot, A. and Hensel, R. P.: "Considerations in Blending Coals to Meet SO₂ Emission Standards," National Coal Association and Bituminous Coal Research, Inc., Coal Conference and Expo III, C-E Power Systems Report TIS-4925 (1976).
4. Beer, J. M.: "International Flame Research Foundation: The Effect of Fineness and Recirculation on the Combustion of Low-Volatile Pulverized Coal," J. Inst. Fuel 37, 286 (1964).
5. Cutress, J. O., Peirce, T. J., and Tucker, A. C. N.: "On the Ignition of Pulverized Anthracite," Combustion and Flame 8, 289 (1964).
6. Corey, R. C.: "Burning Coal in CPI Boilers I: How Coal Properties Influence Handling and Combustion," Chem. Eng., pp. 111-119, Jan. 16, 1978.
7. Reuther, J. J.: "The Role of Sulfur in Combustion," Earth and Mineral Sciences, The Pennsylvania State University (in press).

**APPENDIX I: Pennsylvania State University Proposal to the Jet Propulsion
Laboratory: "Plane Flame Furnace Combustion Tests on
JPL-Desulfurized Coals"**

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Solicited Proposal for the Establishment of a Contract

Submitted to:

Jet Propulsion Laboratory

For Research On:

PLANE FLAME FURNACE COMBUSTION TESTS ON JPL-DESULFURIZED COAL

From:

**The Pennsylvania State University
College of Earth and Mineral Sciences
Department of Materials Science and Engineering
Fuel Science Section
Fuels and Combustion Laboratory**

Principal Investigator: J. J. Reuther (814) 865-4392

Amount Requested: \$10,869

Period of Request: 7/1/81 - 12/31/81

Date of Submission: May 15, 1981

Business Contact: W. D. Moir (814) 863-0587

Submitted by:

Approvals:

**James J. Reuther
Assistant Professor of Fuel Science**

**R. C. Bradt
Head, Department of Materials
Science and Engineering**

**R. G. Cunningham
Vice President for Research and
Graduate Studies**

SUMMARY

Project Title: PLANE FLAME FURNACE COMBUSTION TESTS ON JPL-DESULFURIZED COALS

Principal Investigator: Dr. J. J. Reuther
(814) 865-4392

Assistant Professor of Fuel Science
The Pennsylvania State University
320 Steidle Building
University Park, PA 16802

Project Duration: 7/1/81 - 12/31/81

Estimated Project Budget: \$10,869

Objectives:

To reliably determine, under well-defined and well-controlled simulated boiler combustion conditions, the ignition and burnout characteristics of three (3) samples of raw bituminous rank coal, three (3) samples of the same raw coal partially desulfurized (ca.-60%) by a Jet Propulsion Laboratory (JPL) "chlorination" process, and three (3) samples of the same raw coal more completely desulfurized (ca-85%) by more severe processing with the named JPL technique in order to establish to what extent the burning characteristics of the untreated coals are altered upon sulfur removal.

Research Tasks:

The nine (9) listed samples of pulverized coal with diminishing sulfur content will be fired in The Pennsylvania State University Fuels and Combustion Laboratory plane flame furnace, shown in Figure 1. This intermediate-scale laboratory device essentially simulates the combustion environment in a utility boiler: residence times of 1-2 seconds; peak gas temperatures of 1400-1500°K; heating rates of 10⁴°K/second. Because the furnace design produces a one-dimensional flame, fuel particles experience a nearly identical time/temperature history as they vertically traverse the combustion zone. Flat flames stabilize at different positions downstream of the fuel entry plane primarily because of different compositional properties of the fuel, such as the volatile matter, hydrogen, and fixed-carbon contents. It is the effect of the alteration of these three fuel properties (upon JPL desulfurization: decrease, decrease, and increase, respectively), on raw coal burning characteristics that is to be determined.

The furnace will be fired at 8-10 pounds of pulverized coal (~200 microns) per hour and at + 20% excess air. The Jet Propulsion Laboratory will supply 15-20 pounds of each of the nine samples along with their respective ultimate and proximate analyses.

Flame and wall temperatures and compositions of gaseous and solid products of combustion will be characterized as a function of residence time (downward distance) by sampling the combustion environment through ports distributed along the vertical axis of the furnace. The acquisition of these data will permit the determination of ignition times, burning velocities, and burnout times as a function of coal sample. These data will indicate how well JPL-desulfurized fuels will perform as boiler fuels.

The work statement was developed following detailed discussions with Dr. John Kalvinskis, Project Manager, JPL Coal Desulfurization Program.

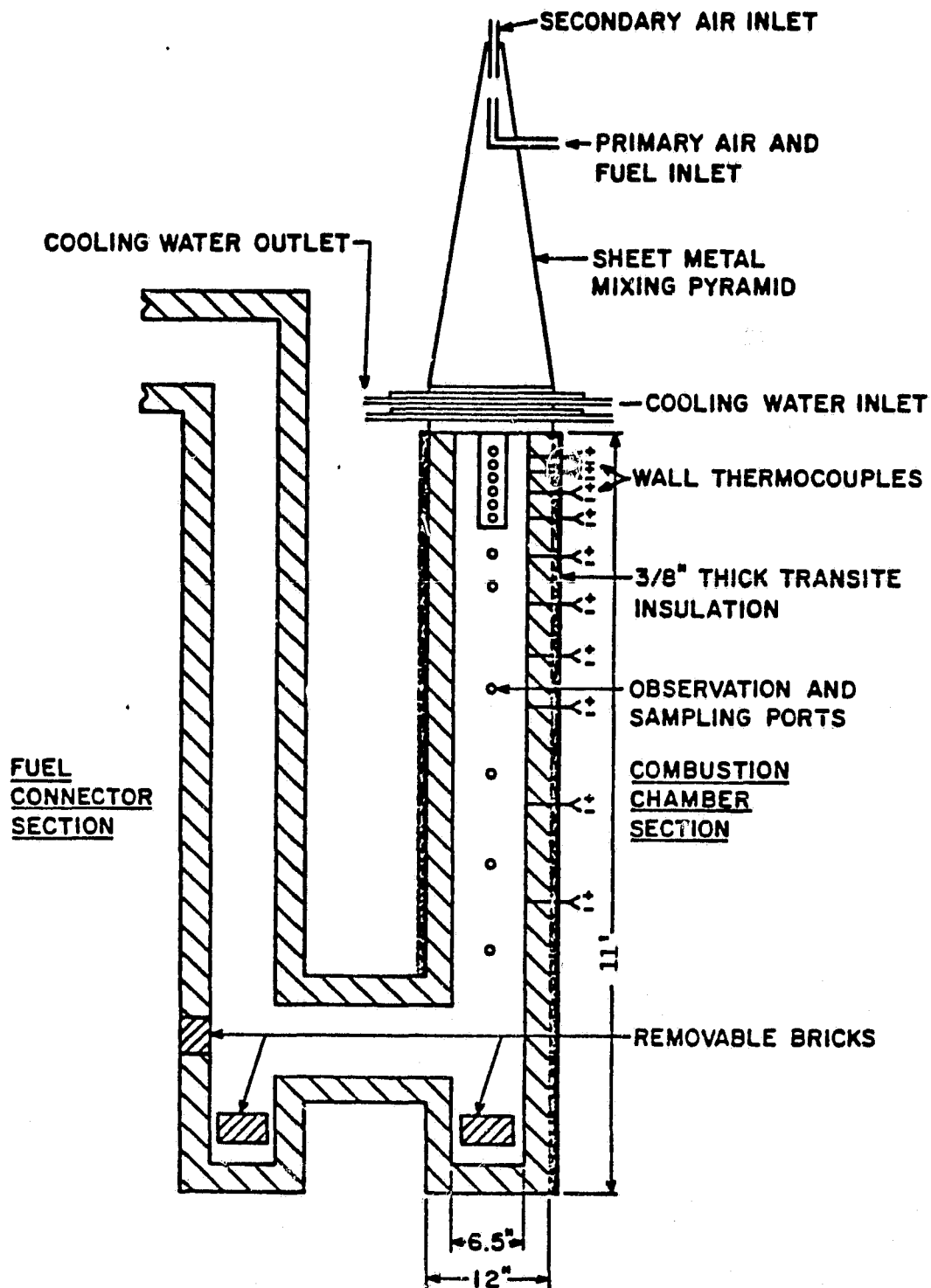


Figure 1. Plane Flame Furnace Schematic

BUDGET ESTIMATE

July 1, 1981 - December 31, 1981

7/1/81-
12/31/81

SALARIES

A. Salaries - (Other than Graduate Assistants)

Principal Investigator, J. J. Reuther @10% time for 6 months	\$1,516
Secretary @ 5% time for 6 months	<u>317</u>
Subtotal of A	\$1,833

B. Salaries - (Graduate Assistants)

Graduate Assistant - @ 50% time for 6 months	\$3,370
Subtotal of B	\$3,370
TOTAL - Salaries and Wages	\$5,203

FRINGE BENEFITS* (see Budget Notes)

23.7% of Salaries (Other than Grad. Assts.)	434
6.8% of Wages and Grad. Asst. Salaries	<u>229</u>
Subtotal - Fringe Benefits	\$ 663

EXPENDABLE SUPPLIES AND EQUIPMENT

Ignition, fire-up fuels; probe parts	<u>1,141</u>
Subtotal - Expendable Supplies and Equipment	\$1,141

OTHER

1. Communications	\$ 100
2. Drafting	100
3. Tuition for Graduate Assistant	<u>1,067</u>
Subtotal - Other	\$1,267

TOTAL DIRECT COSTS	\$8,274
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RECOVERY OF INDIRECT COSTS** (see Budget Notes)

36% (MTDC)	\$2,595
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TOTAL ESTIMATED DIRECT AND INDIRECT COSTS	<u>\$10,869</u>
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BUDGET NOTES

* FRINGE BENEFITS

"Computed at the predetermined fixed rates of 23.7 % applicable to salaries excluding graduate assistant salaries and 6.8 % applicable to wages and graduate assistant salaries for any contract period through June 30, 1982 and subject to redetermination thereafter with such redetermination to coincide with base fiscal periods agreeable to the University and the cognizant Government audit agency involved in making the rate determination."

** INDIRECT COSTS

"Computed at Government approved on Campus rate of 36 % applicable to modified total direct costs (direct costs excluding graduate assistant tuition, amount of individual subcontracts in excess of \$25,000, equipment, plant construction and building amortization) for any contract period through June 30, 1982. For any period subsequent to June 30, 1982 the rate quoted above shall be subject to redetermination to coincide with base fiscal periods agreeable to the University and the cognizant Government audit agency involved in making the indirect cost determinations."

JAMES J. REUTHER

Position: Assistant Professor of Fuel Science (1978)
Fuels and Combustion Laboratory
Department of Materials Science and Engineering

Address: Fuel Science Section
320 Steidle Bldg.
The Pennsylvania State University
University Park, PA 16802
(814) 865-4392

Education: Ph.D. in Fuel Science, The Pennsylvania State University (1979).
Dissertation: "Visible Chemiluminescence From Selected
Low-Pressure Metal Vapor-Oxidant Diffusion Flames"
Advisor: Dr. H. B. Palmer, Professor of Energy Science

M.A. in Flame and Combustion, State University of New York at
Binghamton (1976).
Thesis: "Limiting Equivalence Ratio, Dissociation and
Self-Inhibition in Premixed, Quenched and Fuel-Rich
Hydrocarbon/Air Flames"
Advisor: Dr. W. E. Kaskan, Professor of Chemistry (deceased)
Surrogate Advisor: Dr. D. D. Konowalow, Professor of Chemistry

B.A. in Physical Chemistry, State University College of
New York at Oneonta (1973).

Societies: Sigma Xi, Scientific Research Society
Phi Kappa Phi, Academic Honor Society
Phi Lambda Upsilon, Honorary Chemical Society
The Combustion Institute
American Chemical Society, Divisions of Fuel and Physical Chemistry
American Physical Society, Division of Chemical Physics

Research Interests:

Research in Professor J. J. Reuther's laboratories primarily involves a comprehensive and systematic study of combustion phenomena and how the compositional properties of fuels determine physico-chemical combustion behavior. Various fossil and non-fossil, conventional and alternative, natural and synthetic fueled-flames are being diagnosed, including those of: bituminous, anthracite, and solvent-refined (reconstituted) coal, gasifier char, wood; petroleum, coal-, and shale oil-derived liquids; natural and low-, medium-, and high-Btu gas. By burning, probing, and analyzing flames of a variety of solid, liquid, and gaseous fuels under standardized, well-controlled, and well-defined conditions, Professor Reuther and a team of graduate students intend to achieve a better understanding of the fundamental process of combustion. This information will then be applied to practical combustors in order to delineate ways of burning domestic coal and coal derivatives in an environmentally (air pollution control) and technologically (high efficiencies) acceptable manner. Professor Reuther is also conducting research on the chemical and physical suppression of unwanted combustion e.g., coal dust mine explosions and submerged submarine fires, using solid, liquid, and gaseous agents, and on spectroscopic and mechanistic problems related to chemiluminescent metal atom oxidation reactions.

Publications

Kaskan, W. E. and Reuther, J. J.: "Limiting Equivalence Ratio, Dissociation, and Self-Inhibition in Premixed, Quenched, and Fuel-Rich Hydrocarbon/Air Flames," Sixteenth Symposium (International) on Combustion, pp. 1083-1095, The Combustion Institute, 1977.

Reuther, J. J.: "Comments on Chemical and Physical Inhibition of Quenched and Adiabatic Premixed Flames," Eastern States Section Combustion Institute, Paper IV-31, The Combustion Institute, 1977.

Reuther, J. J.: "Measures of Effectiveness and Mechanisms for Chemical and Physical Inhibition of Quenched and Adiabatic Premixed Flames," Proc. 10th Materials Research Symposium, NBS Special Pub. 561, Vol. 2, pp. 1281-1313, 1979.

Field, R., Gottscho, R. A., Pruett, J. G., and Reuther, James J.: "Barium Oxide: The Questions Unanswered," Free Radicals, Proceedings of Yamada Conference III, The Fourteenth International Symposium, pp. 39-59, Association for Science Documents Information, Japan, 1979.

Ogunsola, O. I., Isles, G. L., and Reuther, J. J.: "The Effect of Increased Aromaticity on the Combustion Characteristics of Paraffinic Kerosine," Central States Section Combustion Institute Meeting on Combustion and Utilization of Alternative Fuels, CSS/CI-80-05 (1980).

Reuther, J. J.: "Combustion of Alternative Natural and Synthetic Fuels," Earth and Mineral Sciences 49:5, 49, 57-59, The Pennsylvania State University (1980).

Ogunsola, O. I. and Reuther, J. J.: "Relationship Between Fuel-Nitrogen-to-NOX Conversion Efficiency and Boiling Range for Coal-Derived Liquid Fuel Combustion," Eastern States Section Combustion Institute, Paper 12, The Combustion Institute, 1980.

RESEARCH PROGRAMS OF PROFESSOR J. J. REUTHER
PENNSYLVANIA STATE UNIVERSITY FUELS AND COMBUSTION LABORATORY
(Advanced Fuel Science Degree Candidates)

COMBUSTION/INHIBITION PHYSICO-CHEMISTRY OF COAL-DERIVED SYNGAS/AIR FLAMES

J. Withum (Ph.D.); R. Daley (M.S.)

Fuels [CH_4 , CO , H_2 , NH_3] and diluents [CO_2 , H_2O , N_2] will be mixed together with the compositions of commercial, coal-derived gases simulated. The physical [temperatures] and chemical [species concentrations] microstructures of non-adiabatic flat syngas/air flames will be determined. The objectives are: a) to gather combustion data on alternate syngases; b) to decipher how CO_2 and H_2O act to extinguish flames, and c) to determine whether secondary/tertiary fuel and/or diluent affect NOX and smoke production/destruction.

COMBUSTION CHARACTERISTICS OF ALTERNATIVE LIQUID FUELS

O. Ogunsola (Ph.D.)

Coal liquids, shale oils, and doped and neat petroleum fuel oils will be fired at 10^6 Btu/hr and at $\pm 15\%$ excess air in a hot-wall furnace. The objective is to systematically and comprehensively determine and model the relationships among the alternative liquid fuel compositional properties and the thermal (radiative heat transfer; combustion efficiency) and chemical (NOX, smoke pollution potential) combustion performance of the furnace in order to assess the feasibility of substituting coal- and shale oil-derived liquids for petroleum-based fuels.

COMBUSTION OF ANTHRACITE AND SOLVENT REFINED COAL, GASIFIER CHAR, AND WOOD

C. Macey (Ph.D.)

Selected anthracite and solvent refined coals, gasifier chars, and wood will be fired in a laboratory plane flame furnace that essentially simulates the combustion environment in a utility boiler. Combustion data will be used to delineate the relationships between the composition properties of natural and synthetic solid fuels and their respective thermal (ignition, burnout) and chemical (NOX, SOX, particulate pollution potential) combustion performance, and to evaluate the economic, environmental, and strategic consequences of replacing conventional bituminous boiler fuels with the named alternatives.

FORMATION OF SOOT IN RICH HYDROCARBON COMBUSTION

J. Warchol (M.S.)

Gas-phase carbon formation/destruction rates and mechanisms will be determined in the high-temperature environments produced by a laminar flat flame burner and a turbulent plug-flow reactor as a function of fuel [current/future hydrocarbon precursors to fuel-cell fuel (H_2)], stoichiometry [from very fuel-rich flames to pure pyrolysis], additive/diluent [potential soot suppression agents such as H_2O], and at simulated hydrocarbon-reformer conditions [~ 1000 - $1400^\circ K$; ~ 1 atm].

COAL DUST/AIR EXPLOSION AND SUBMARINE FIRE SUPPRESSION USING WATER, INORGANIC POWDERS, AND HYBRIDS OF THESE AGENTS

H. Kim (Ph.D.); P. Taylor (Ph.D.)

A laminar quenched flat-flame [perforated] burner will be used to generate variable residence time/temperature histories that essentially simulate the conditions existing in coal mine dust explosions [1100 - $1500^\circ K$], mine face gas ignitions [1500 - $1800^\circ K$] and submerged submarines fires. The objectives are to: a) determine how effectively water, inorganic powders [eg., $KHCO_3$, $NH_4H_2PO_4$], and aqueous salt solutions suppress unwanted combustion in coal-winning and defense operations, b) elucidate the chemical-physical inhibition mechanism, and c) design more effective, second-generation agents.

CHEMILUMINESCENT REACTIONS OF METAL VAPORS

J. J. Reuther

Spectroscopic and mechanistic studies are conducted on visible-chemiluminescent gas-phase atom-transfer reactions involving a variety of metals [eg., Ba, Sr, Ca, Sn, B] and oxidants [eg., N_2O , O_3 , ClO_2 , O_2]. The objective is to provide a more complete, systematic, and detailed understanding of the events that determine [e.g., spin conservation, exothermicity] and control [e.g., collision-induced transfer processes] the identities and light production efficiencies [photon yield] of electronically-excited metal oxides.

**APPENDIX II: Advance Report of Final Results on PSU Combustion Tests
on JPL-Desulfurized Coals**

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THE PENNSYLVANIA STATE UNIVERSITY

FUELS AND COMBUSTION LABORATORY
UNIVERSITY PARK, PENNSYLVANIA 16802

College of Earth and Mineral Sciences
Fuel Science Section
Department of Materials Science & Engineering

May 7, 1982

Area Code: 814
863-4392
863-4802

Dr. John J. Kalvinskas
Project Manager Coal Desulfurization
Jet Propulsion Laboratory
Mail Code 125159
4800 Oak Grove Drive
Pasadena, Ca 91109

Dear John:

In the interest of delivering the essential results from our final plane flame furnace combustion tests on raw and JPL-desulfurized coals to you with dispatch and in advance of our submission of a draft final report (PSU-FCL-C-82-345), I have prepared the following table of contract-required data and more:

No.	Coal	Process	Volatile Matter (%)	Ignition Time (msec)	Burning Velocity (cm/sec)	Burnout Time (msec)	Flame Length (cm)
1	PSOC-282	Raw	33.8	3	31.3	239	40.3
2	PSOC-282	CL	25.1	64	28.1	266	44.8
3	PSOC-282	CL/HDS	7.6	201	23.2	322	54.3
4	PSOC-276	Raw	37.2	3	32.8	228	38.4
5	PSOC-276	CL	23.2	76	27.5	272	45.8
6	PSOC-276	CL/HDS	6.5	210	23.0	325	54.8
7	PSOC-230	Raw	38.9	2	33.7	222	37.4
8	PSOC-230	CL	34.2	3	31.6	237	39.9
9	PSOC-230	CL/HDS	6.3	212	22.9	326	54.9

Some succinct definitions are required for clarity: CL-Chlorinolysis processed; CL/HDS = chlorinated and hydrodesulfurized; ignition time = the residence time required for 1% coal carbon burnoff; burnout time = the residence time required for 100% carbon burnoff. Full details of how these data were experimentally generated are, of course, given in the final report. The volatile matter content of the nine test coals correlates well with their respective combustion performance characteristics, as expected; that is why this information has been included in the table.

The trends for the results are not too surprising: as the volatile matter content decreases, ignition time is delayed, burning velocity or overall reaction rate decreases, and burnout time is lengthened. The table quantifies this behavior. The major reason for the generic two-fold increase in burnout time upon chlorination/hydrodesulfurization rests primarily on ignition phenomena: coal No. 1, 4, 7, and 8 exhibited zero ignition delay times, whereas the others had ignition delay

Dr. John J. Kalvinskus
Page 2
May 7, 1982

times that dominated (~95%) ignition times. Once ignited, the lowest volatile coals burned quite well; chlorinated and hydrodesulfurized high-sulfur coal (Nos. 3, 6, 9) flame lengths were only ca. 50% longer than the parent raw coals they were derived from.

As I will address in the draft final report, burner technology exists that may help to circumvent the ignition delay problem for the severely desulfurized coals. Other promising ways to utilize JPL-desulfurized coals will also be evaluated.

I hope that this dashed-off letter satisfies your immediate needs. The draft report will be forthcoming.

With best wishes.

Sincerely yours,

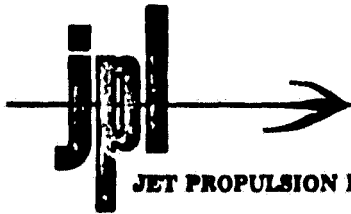


James J. Reuther
Assistant Professor of Fuel Science

JJR:blg

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APPENDIX III: JPL Test Coal Analyses



JET PROPULSION LABORATORY *California Institute of Technology • 4800 Oak Grove Drive, Pasadena, California 91103*

April 9, 1982

Refer to JK:dy-TRSE-345-4

Dr. James Reuther
The Pennsylvania State University
207 Old Main Building
University Park, PA 16802

Dear Jim:

I have enclosed analyses we have received from the Colorado School of Mines Research Institute for the six batches of desulfurized coal. The analyses include sulfur forms, proximate and ultimate analyses.

I have marked the coal samples that were treated without hydrodesulfurization by an asterisk with that notation. Three coal samples were included in that category. The three coal samples that were treated with hydrodesulfurization are marked accordingly.

I hope this information is helpful to you in your interpretation of the combustion tests. If you have any questions, please call at (213) 354-2349.

Sincerely,


John J. Kalvinskas, Ph.D.
Project Manager

xc: R. Phen
G. Varsi

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Jet Propulsion Laboratory
California Institute of Technology
4800 Oak Grove Drive
Pasadena, CA 91100

Colorado School of Mines Research Institute

Project No. A20106
JPL P.O. #RD-152, Job #763-10903-0-3450

Page 1 of 3

March 8, 1982

P.O. BOX 112 • GOLDEN, COLORADO 80401
PHONE (303) 279-2581 • TWX 910-504-0184 • CSM Res Cdn



Sample	Moisture	ASH %		VOLATILE MATTER %		FIXED CARBON %		BTU/LB		CARBON %		HYDROGEN %		NITROGEN %	
		(AD)	(DRY)	(AD)	(DRY)	(AD)	(DRY)	(AD)	(DRY)	(AD)	(DRY)	(AD)	(DRY)	(AD)	(DRY)
Run 9 PLM	0.80	25.8	26.0	8.72	8.79	64.7	65.2	10844	10931	65.5	66.0	2.56	2.49	1.21	1.22
Run 10 ILL	1.12	10.3	10.4	9.38	9.49	79.2	80.1	13138	13282	81.4	82.3	3.08	2.99	1.41	1.43
Run 11 ILL	0.91	10.7	10.8	10.2	10.3	78.2	78.9	13115	13233	79.8	80.5	3.09	3.02	1.60	1.61
PSOC 230 *	0.61	9.73	9.79	34.0	34.2	55.7	56.0	12055	12127	76.6	77.1	4.18	4.14	1.10	1.11
PSOC 276 *	0.48	9.83	9.88	23.4	23.5	66.3	66.6	12728	12792	72.3	72.7	3.96	3.93	1.45	1.46
PSOC 282 *	0.71	7.70	7.76	24.9	25.1	66.7	67.2	12969	13060	76.7	77.2	3.97	3.92	1.82	1.83

Sample	CHLORINE %	
	(AD)	(DRY)
Run 9	0.35	0.35
Run 10	0.46	0.46
Run 11	0.45	0.45
PSOC 230 *	0.74	0.74
PSOC 276 *	1.12	1.13
PSOC 282 *	2.84	2.86

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Stanley D. Schoenwald

Stanley D. Schoenwald
Supervisor, Coal Laboratory

* CHLORINOLYSIS PROCESSED
COALS WITHOUT HYDROGEN SULFIDE REMOVAL

March 8, 1982

P.O. BOX 112 • GOLDEN, COLORADO 80401
PHONE (303) 279-2581 • TWX 910-934-0194 • CSM Res Gdn

Sample	ASTM FORMS OF SULFUR									
	TOTAL		SULFATE		PYRITIC		ORGANIC		OXYGEN %	
	SULFUR %		SULFUR %		SULFUR %		SULFUR %		(AD) (DRY)	
	(AD)	(DRY)	(AD)	(DRY)	(AD)	(DRY)	(AD)	(DRY)	(AD)	(DRY)
Run 9 PCH #8	0.42	0.42	<0.05	<0.05	0.02	0.02	0.40	0.40	4.16	3.48
Run 10 ILL #6	1.09	1.10	<0.05	<0.05	<0.01	<0.01	1.10	1.10	2.26	1.28
Run 11 EAGLE #5	0.30	0.30	<0.05	<0.05	<0.01	<0.01	0.30	0.30	4.06	3.28
PSOC 230 *	0.62	0.62	<0.05	<0.05	0.24	0.24	0.38	0.38	7.03	6.53
PSOC 276 *	1.30	1.31	<0.05	<0.05	0.14	0.14	1.16	1.17	10.0	9.62
PSOC 282 *	0.68	0.68	<0.05	<0.05	0.15	0.15	0.53	0.53	6.29	5.70

* CHLORINOLYSIS PROCESSED
COAL WITHOUT HYDRODESULFURIZATION

Stanley D. Schoenwald
Supervisor, Coal Laboratory

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Colorado School of Mines Research Institute

Jet Propulsion Laboratory
Project No. A20106

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March 8, 1982

Page 3 of 3

SAMPLE	CHLORINE %		RECALCULATED OXYGEN %	
	(AD)	(DRY)	(AD)	(DRY)
3	<0.05	<0.05	2.73	1.47
4	0.07	0.07	2.38	1.29
5	<0.05	<0.05	2.50	1.27
6A	0.16	0.16	2.70	2.31
6B	0.07	0.07	2.18	1.64
6C	<0.05	<0.05	2.26	1.76

Stanley D. Schoenwald
Stanley D. Schoenwald
Supervisor, Coal Laboratory

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ab

Colorado School of Mines Research Institute

Jet Propulsion Laboratory
California Institute of Technology
4800 Oak Grove Drive
Pasadena, CA 91109

April 5, 1982

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CSM RI

Project No. A20106
Page 1 of 2

Sample	Moisture %	Ash % <u>(AD)</u> <u>(DRY)</u>	Volatile Matter % <u>(AD)</u> <u>(DRY)</u>	Fixed Carbon % <u>(AD)</u> <u>(DRY)</u>	BTU/LB <u>(AD)</u> <u>(DRY)</u>	Carbon % <u>(AD)</u> <u>(DRY)</u>	Hydrogen % <u>(AD)</u> <u>(DRY)</u>
PSOC 230 Chlorinated and Hydrodesulfur- ized	0.82	11.9	6.20	6.25	81.1	81.8	2.14
PSOC 276 Chlorinated and Hydrodesulfur- ized	0.82	8.56	6.45	6.50	84.2	84.9	2.07
PSOC 282 Chlorinated and Hydrodesulfur- ized	1.18	10.0	7.48	7.57	81.3	82.3	2.13

Sample	Nitrogen % <u>(AD)</u> <u>(DRY)</u>	Chlorine % <u>(AD)</u> <u>(DRY)</u>
PSOC 230 Chlorinated and Hydrodesulfur- ized	1.19 1.20	0.49 0.49
PSOC 276 Chlorinated and Hydrodesulfur- ized	1.72 1.73	0.50 0.50
PSOC 282 Chlorinated and Hydrodesulfur- ized	1.73 1.75	1.57 1.59

Stanley D. Schoenwald
Stanley D. Schoenwald
Coal Laboratory Supervisor

Jet Propulsion Laboratory

Project No. A20106
Page 2 of 2

Colorado School of Mines Research Institute

April 5, 1982

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CSM

Sample	ASTM FORMS OF SULFUR									
	Total Sulfur % <u>(AD)</u> <u>(DRY)</u>	SO ₄ Sulfur % <u>(AD)</u> <u>(DRY)</u>	Pyritic Sulfur % <u>(AD)</u> <u>(DRY)</u>	Organic Sulfur % <u>(AD)</u> <u>(DRY)</u>	Oxygen % <u>(AD)</u> <u>(DRY)</u>					
PSOC 230 Chlorinated and Hydrodesulfur- ized	0.38	0.38	<0.05	<0.05	0.01	0.01	0.37	0.37	3.53	2.82
PSOC 276 Chlorinated and Hydrodesulfur- ized	0.53	0.53	<0.05	<0.05	0.04	0.04	0.49	0.49	2.85	2.14
PSOC 282 Chlorinated and Hydrodesulfur- ized	0.32	0.32	<0.05	<0.05	0.05	0.05	0.27	0.27	3.14	2.12

Stanley D. Schoenwald

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Coal Laboratory Supervisor

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OF POOR QUALITY

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